

=> b reg

FILE 'REGISTRY' ENTERED AT 17:08:17 ON 21 APR 2004
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STRUCTURE FILE UPDATES: 19 APR 2004 HIGHEST RN 676225-08-4
DICTIONARY FILE UPDATES: 19 APR 2004 HIGHEST RN 676225-08-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

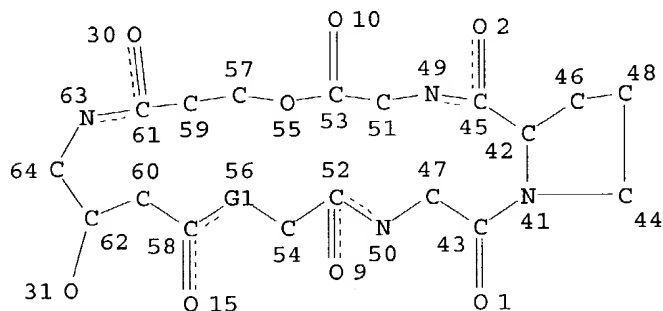
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d que 157
L57

STR



VAR G1=N/O

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

=> b hcaplus

FILE 'HCAPLUS' ENTERED AT 17:08:30 ON 21 APR 2004
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FILE COVERS 1907 - 21 Apr 2004 VOL 140 ISS 17
FILE LAST UPDATED: 20 Apr 2004 (20040420/ED)

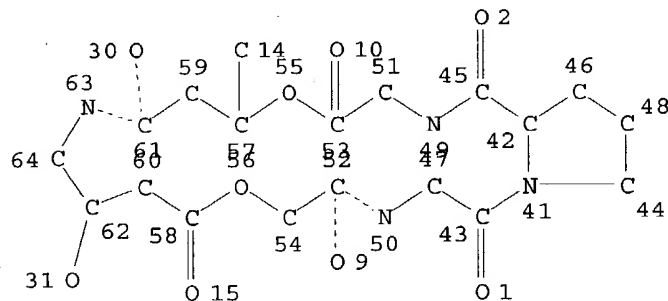
This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que 162

L53

STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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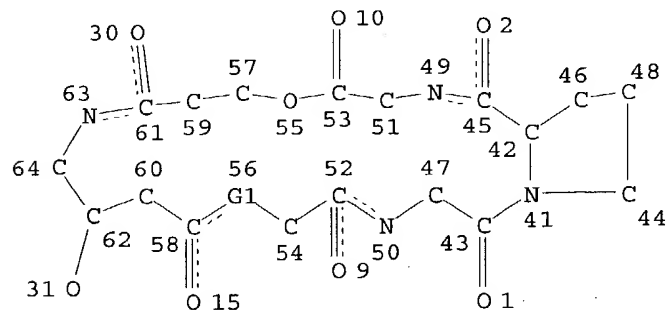
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STEREO ATTRIBUTES: NONE

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L56 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L55

L57 STR



VAR G1=N/O

NODE ATTRIBUTES:

Searched by P. Ruppel

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

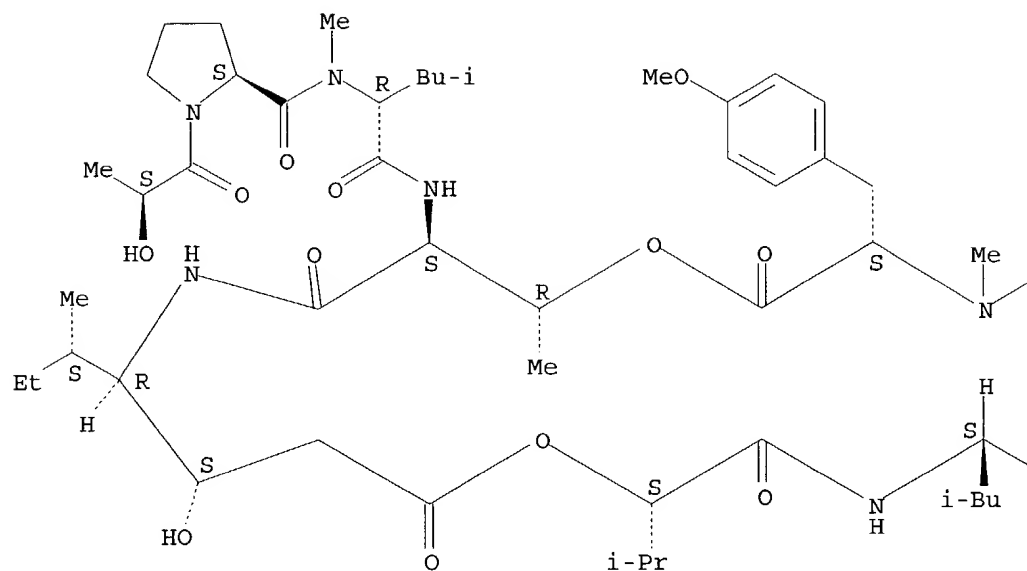
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L61 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L60
L62 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L56 OR L61

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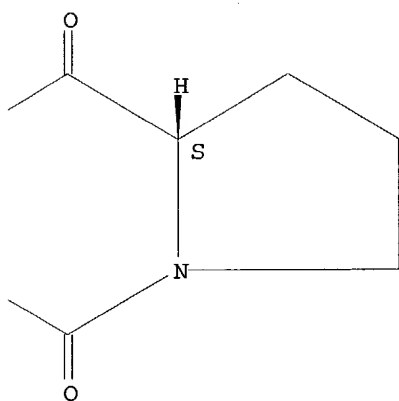
L62 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:898771 HCAPLUS
DOCUMENT NUMBER: 138:86871
TITLE: Chemical defense in ascidians of the Didemnidae Family
AUTHOR(S): Joulle, Madeleine M.; Leonard, Michael S.; Portonovo,
Padma; Liang, Bo; Ding, Xiaobin; La Clair, James J.
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,
Philadelphia, PA, 19104-6323, USA
SOURCE: Bioconjugate Chemistry (2003), 14(1), 30-37
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Fluorescent analogs (DB1 and TA1) of the secondary metabolites didemnin B
(DB) and tamandarin A (TA) were synthesized to investigate the potential
chemical defense mechanisms of tunicates in the family Didemnidae. These
compsds. were found to alter predator-prey relations. Five species of
freshwater fish and one marine fish, the damselfish Amphiprion ocellaris,
were acclimated to a diet of mosquito larvae. Fish showed an immediate,
neg. reaction to mosquito larvae treated with ≥ 5 ng of DB1 or TA1,
with consumption of larvae resulting in regurgitation. Both freshwater
and marine fish learned to avoid tainted prey by associating species of larvae
with "distaste". Distaste for a given organism also arose when
depsipeptides DB1 or TA1 were transferred to the fish from the surrounding
medium. Fluorescence microscopy in fish indicated that a similar
processing and localization followed ingestion and absorption of DB1 or
TA1. Fluorescent labeling of DB or TA provided an ideal tool to conduct
short-term studies of predator-prey relationships between fish and marine
invertebrate larvae.
IT 250211-78-0, Tamandarin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(chemical defense mechanisms of tunicates)
RN 250211-78-0 HCAPLUS
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



IT 485389-87-5

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
(Uses)

(tamandarin A fluorescent analog; chemical defense mechanisms of
tunicates)

RN 485389-87-5 HCAPLUS

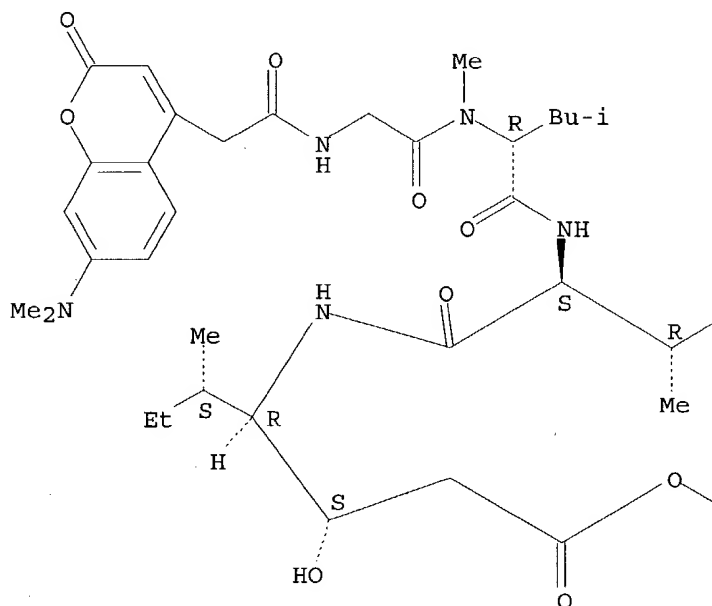
CN L-Tyrosine, N-[[7-(dimethylamino)-2-oxo-2H-1-benzopyran-4-yl]acetyl]glycyl-
N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-

Searched by P. Ruppel

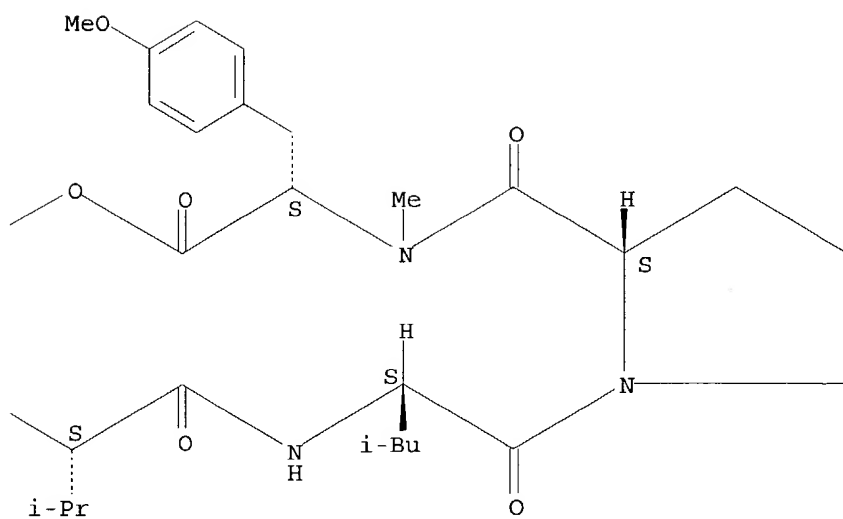
methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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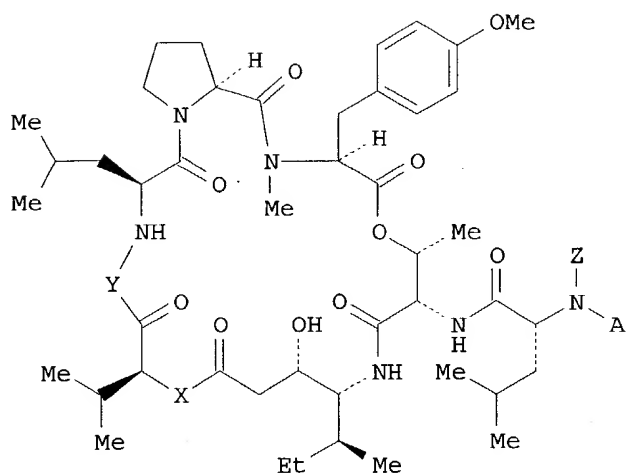
37

THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Searched by P. Ruppel

L62 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2002:31485 HCAPLUS
 DOCUMENT NUMBER: 136:86058
 TITLE: Preparation of aplidine analogs as new antitumor agents
 INVENTOR(S): Rodriguez, Ignacio; Polanco, Concepcion; Cuevas, Felix; Mandez, Paloma; Cuevas, Carmen; Gallego, Pilar; Munt, Simon; Manzanares, Ignacio
 PATENT ASSIGNEE(S): Pharma Mar, S.A., Spain
 SOURCE: PCT Int. Appl., 241 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002596	A2	20020110	WO 2001-GB2901	20010702
WO 2002002596	A3	20020523		
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RW:				
GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1294747	A2	20030326	EP 2001-945484	20010702
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001012375	A	20030624	BR 2001-12375	20010702
JP 2004502702	T2	20040129	JP 2002-507848	20010702
NO 2002006242	A	20030227	NO 2002-6242	20021227
PRIORITY APPLN. INFO.:			GB 2000-16148	A 20000630
			GB 2001-3750	A 20010215
			WO 2001-GB2901	W 20010702
OTHER SOURCE(S):		CASREACT 136:86058; MARPAT 136:86058		
GI				



I

AB Aplidine and its analogs I [$X = CH_2$, O, S, or NR_1 , where $R_1 = H$, (un)substituted alkyl, alkenyl, aryl, aralkyl; $Y = (COR_2)_nCO$, where $n = 0$ or 1, $R_2 = (un)substituted$ alkyl, alkenyl, aryl, aralkyl; $Z = H$, or R_3CONH , R_3CO , where $R_3 = (un)substituted$ alkyl, alkenyl, aryl, aralkyl; $A = amino$ acyl, R_3SO_2 , or R_3CO , where $R_3 = (un)substituted$ alkyl, aryl, aralkyl] were prepared as antitumor agents. Thus, [Val]₃[Isobutyryl]₈-didemnin A was prepared by multistep procedure starting from reaction of H-Leu-Pro-OCH₂Ph with Boc-Val-OH (Boc = tert-butoxycarbonyl) and via coupling of Ist-Val-Leu-Pro-OBn (Ist = isostatine) intermediate with O-(Cbz-N,O-dimethyl-Tyr)-N-tert-Boc-Thr phenacyl ester (Cbz = benzyloxycarbonyl), followed by macrocyclization and coupling with Cbz-Me-D-Leu and Pyr-Pro-OH. The prepared compound was active against human lung carcinoma and human colon carcinoma.

IT 250211-78-0P, Tamandarin A 367507-55-9P

387823-42-9P 387823-43-0P 387823-44-1P

387823-45-2P 387823-56-5P 387823-59-8P

387823-61-2P 387823-62-3P 387823-82-7P

387823-84-9P 387823-85-0P 387823-86-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

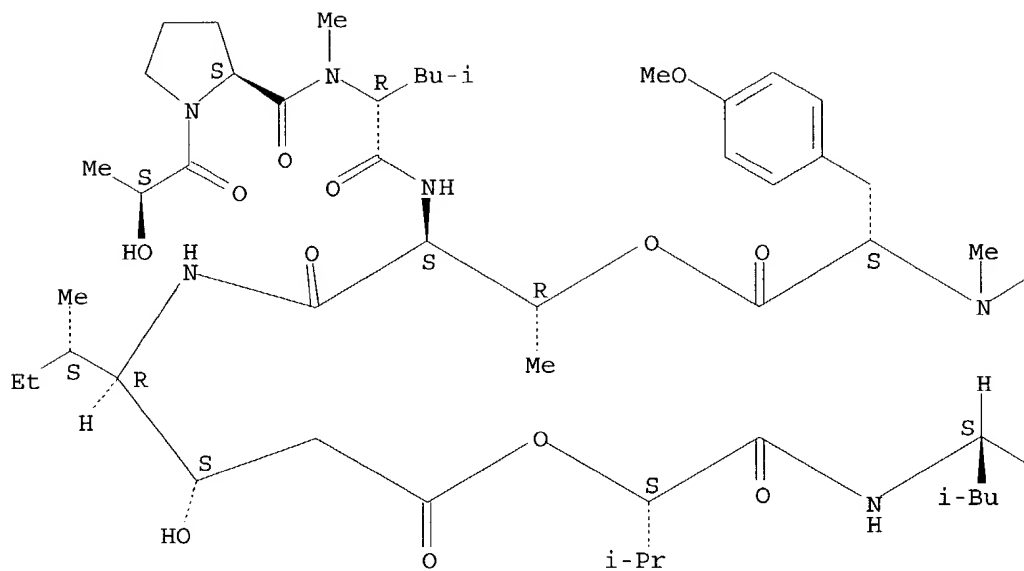
(preparation of aplidine analogs as antitumor agents)

RN 250211-78-0 HCAPLUS

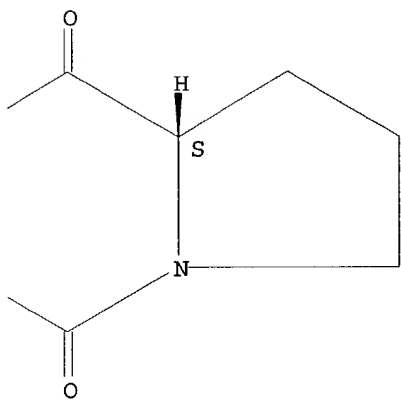
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B

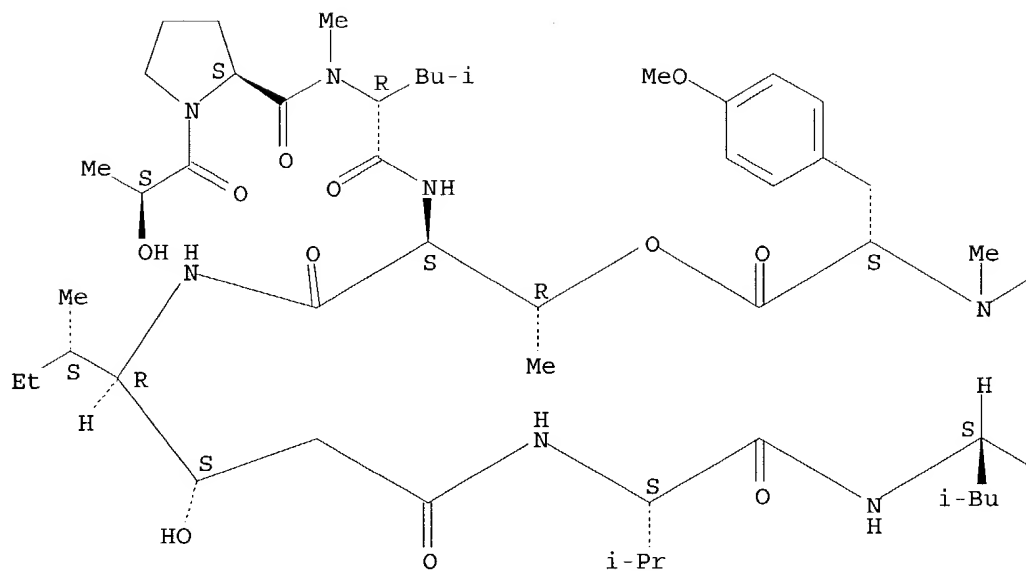


RN 367507-55-9 HCAPLUS
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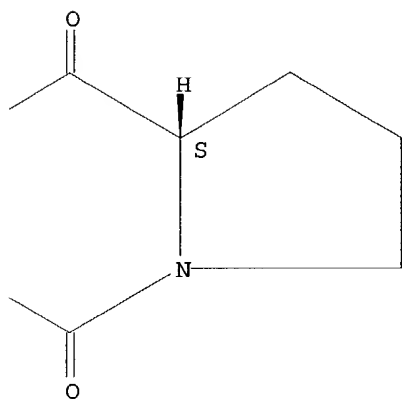
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B

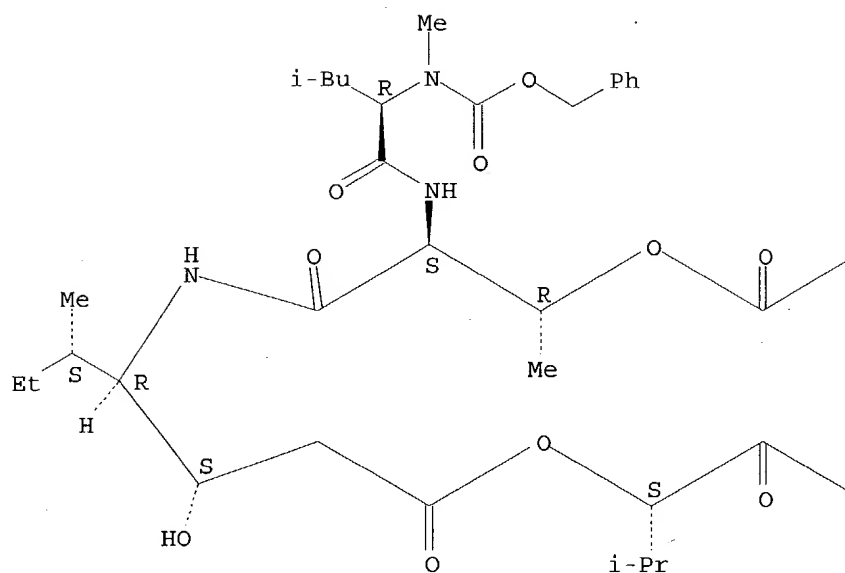


RN 387823-42-9 HCAPLUS
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 (CA INDEX NAME)

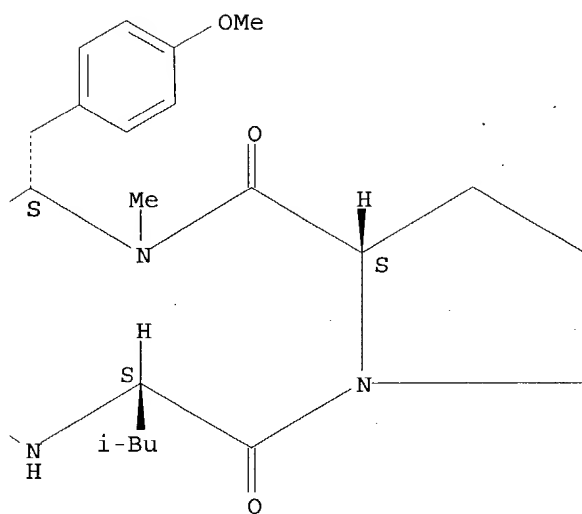
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



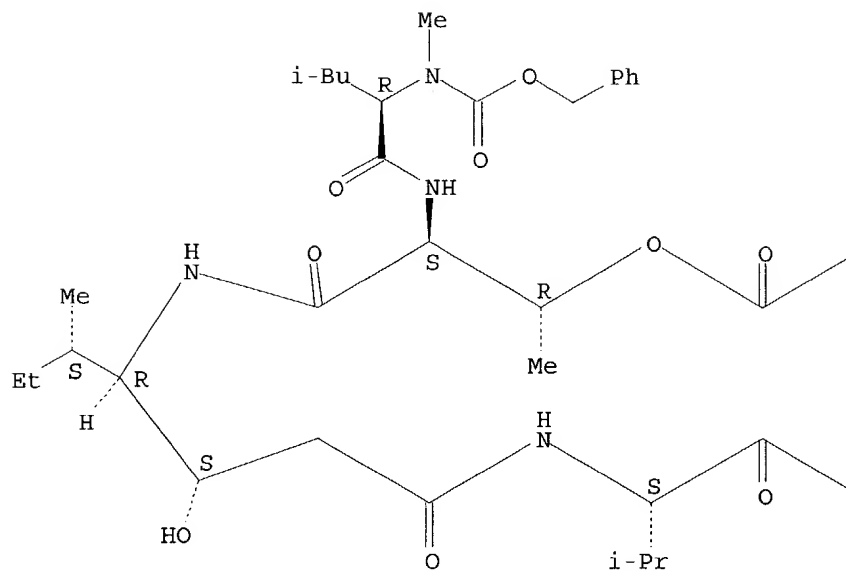
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CN L-Tyrosine, N-methyl-N-[(phenylmethoxy)carbonyl]-D-leucyl-L-threonyl-
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 N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

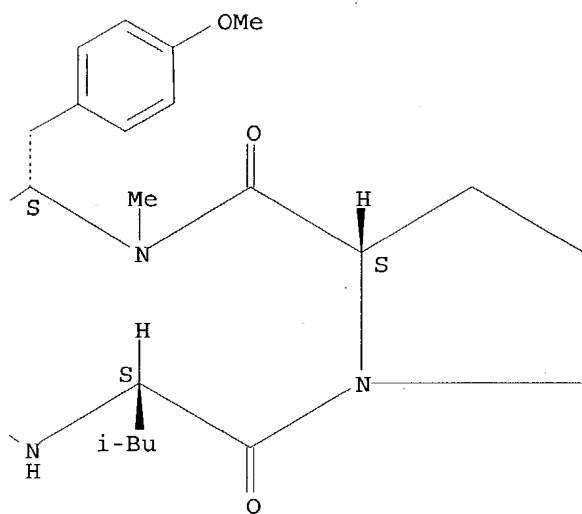
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



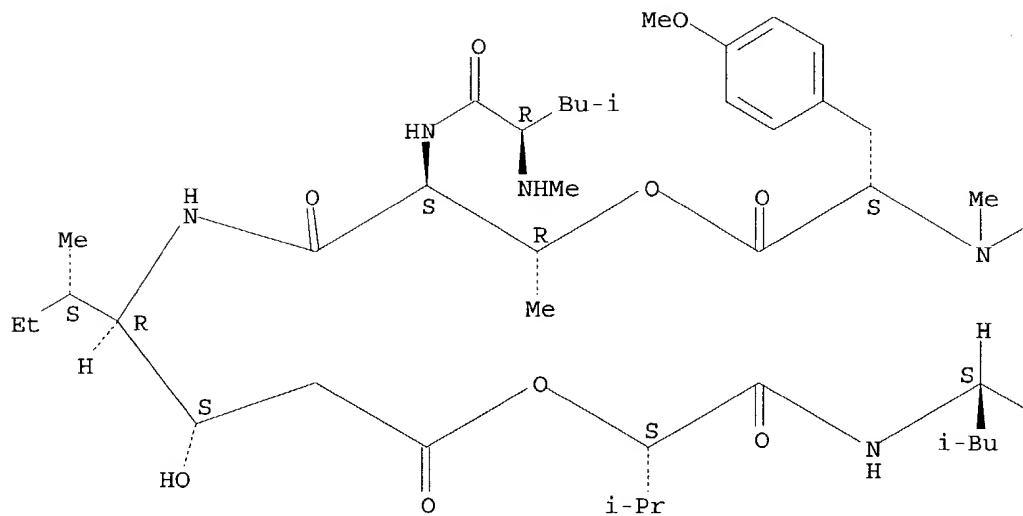
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CN L-Tyrosine, N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

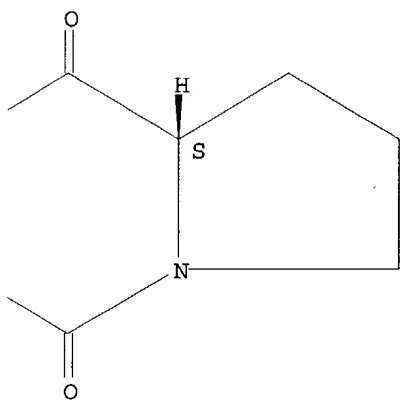
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



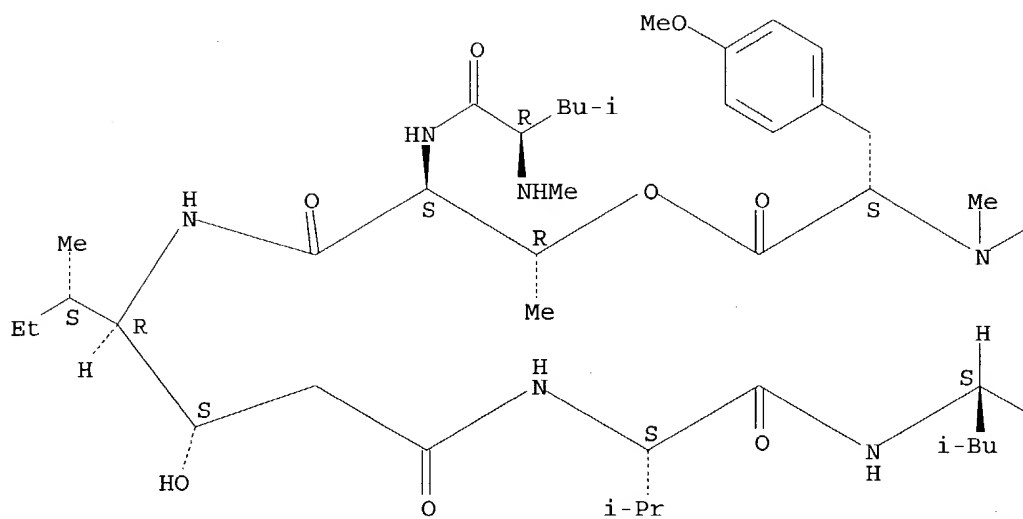
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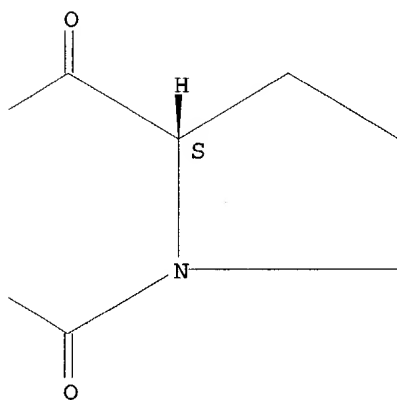
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Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



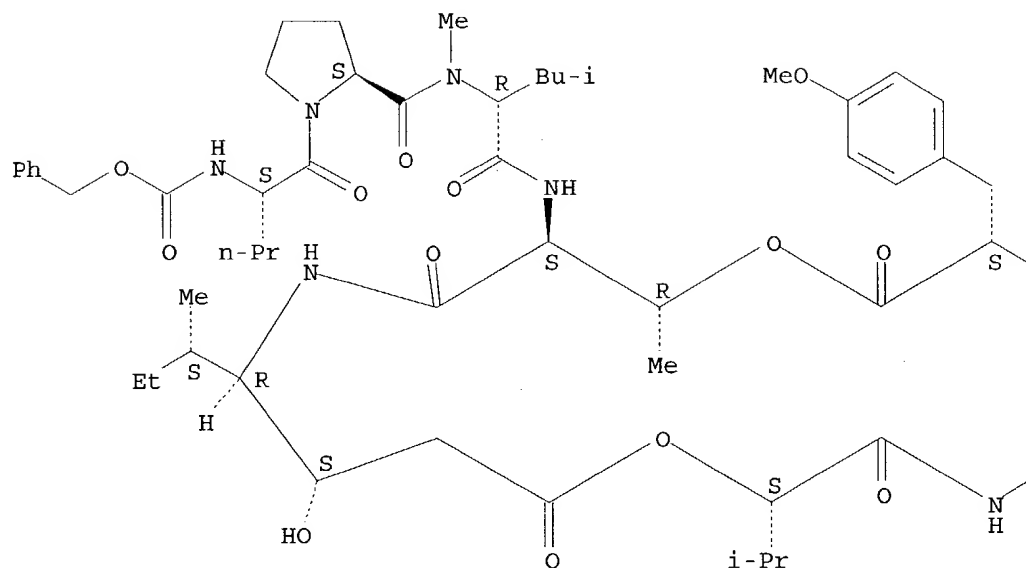
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CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]-L-norvalyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

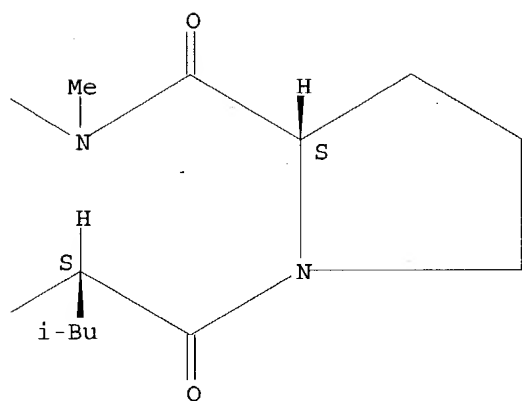
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



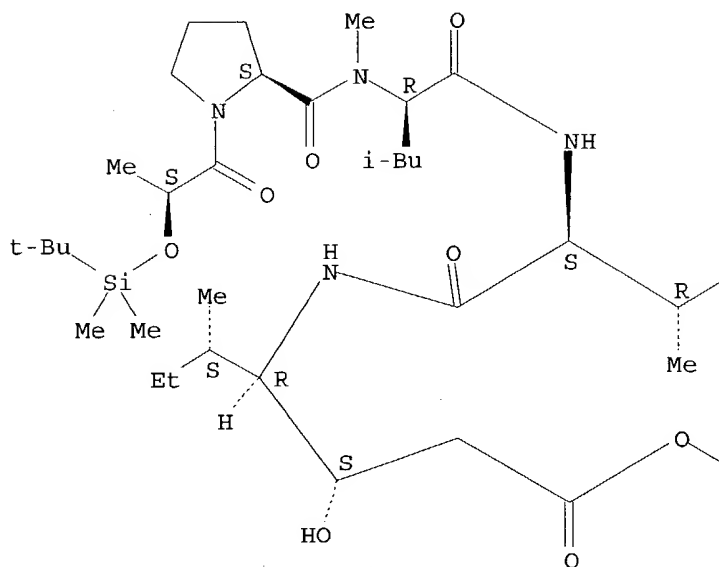
RN 387823-59-8 HCAPLUS

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 dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

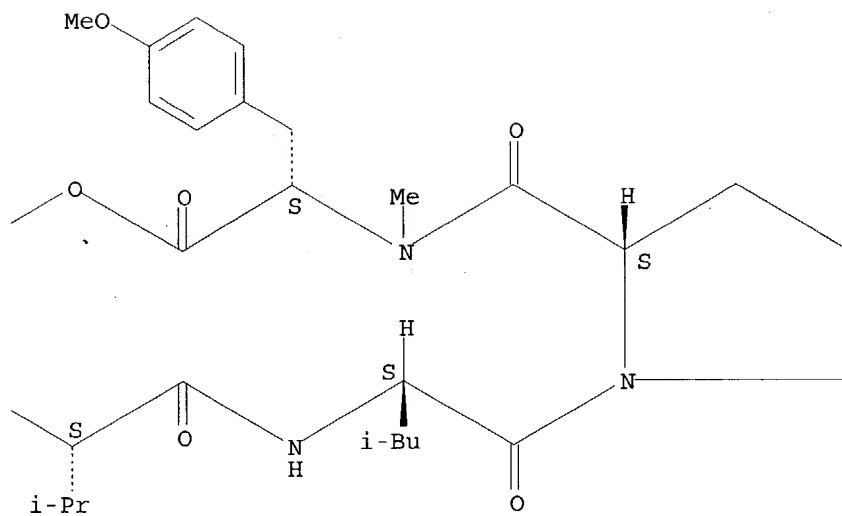
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



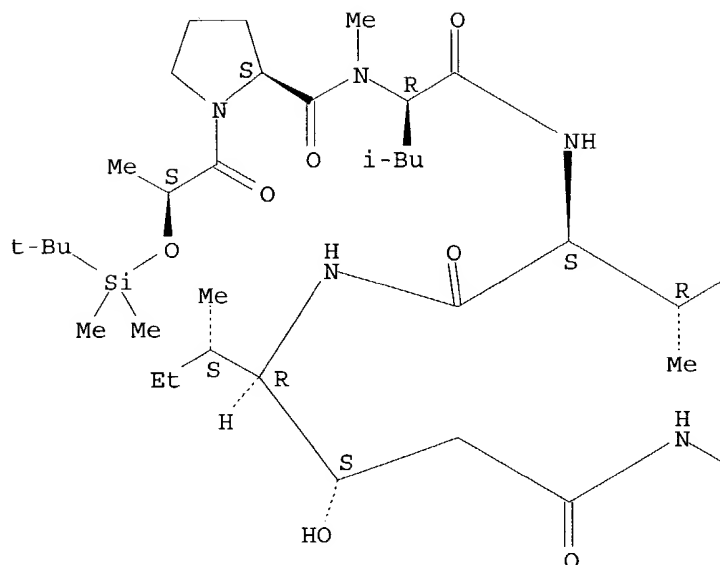
RN 387823-61-2 HCAPLUS

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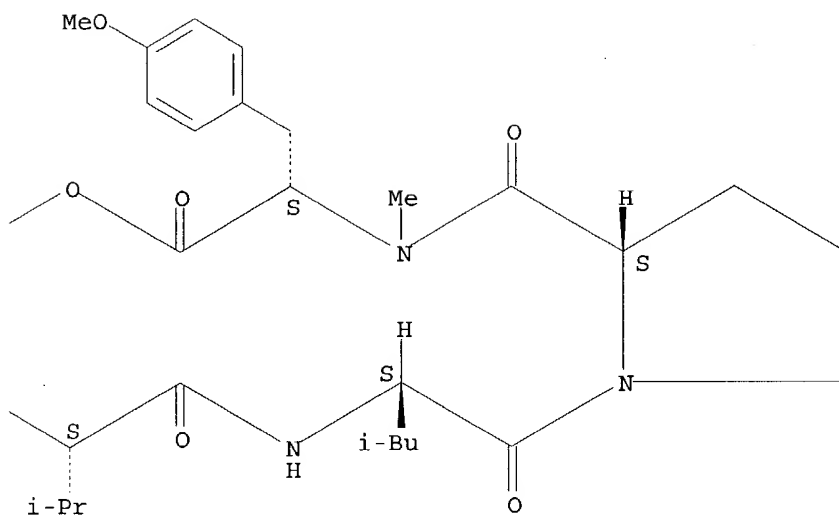
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



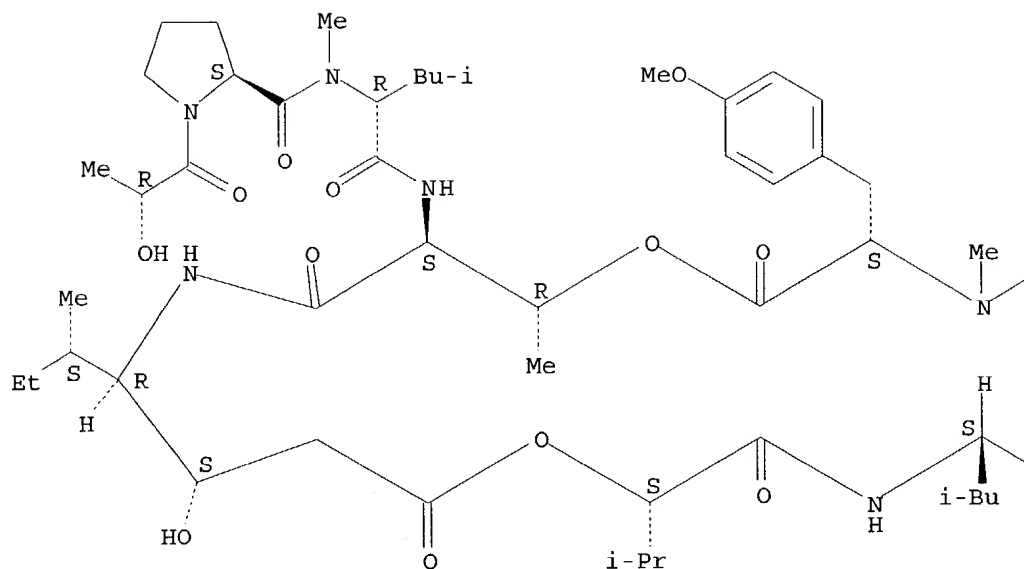
RN 387823-62-3 HCAPLUS

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 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-
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 (CA INDEX NAME)

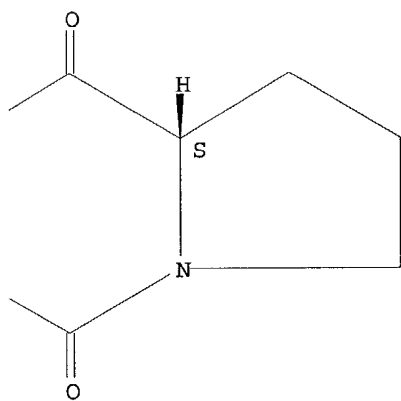
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



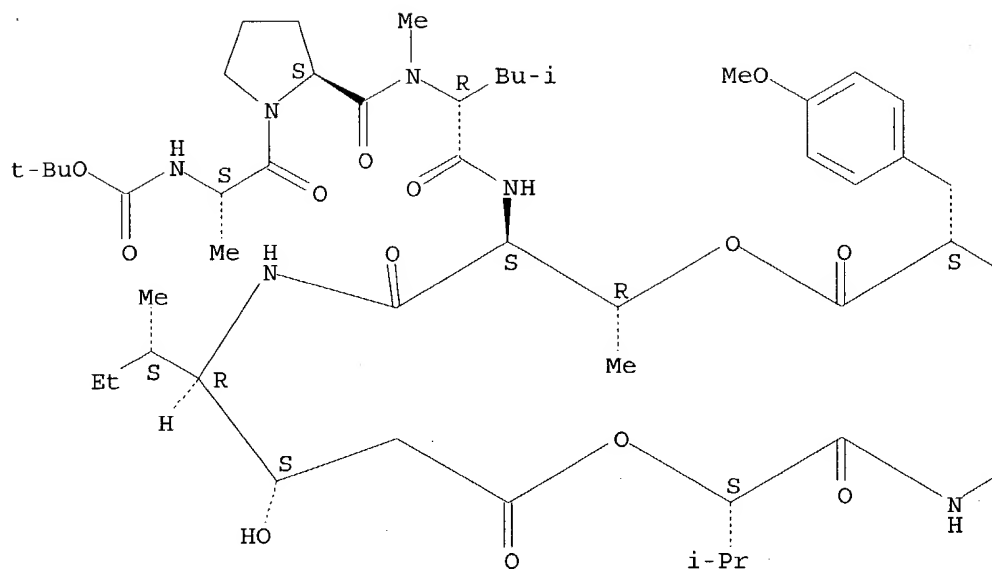
RN 387823-82-7 HCAPLUS

CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

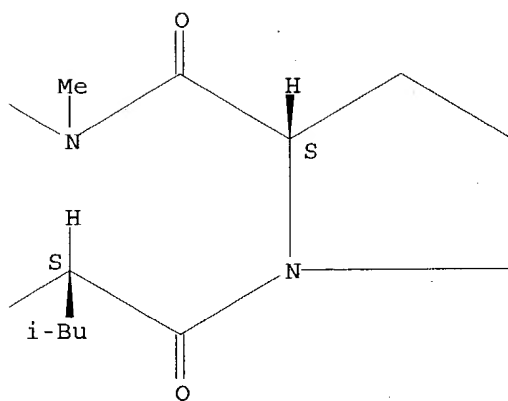
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B

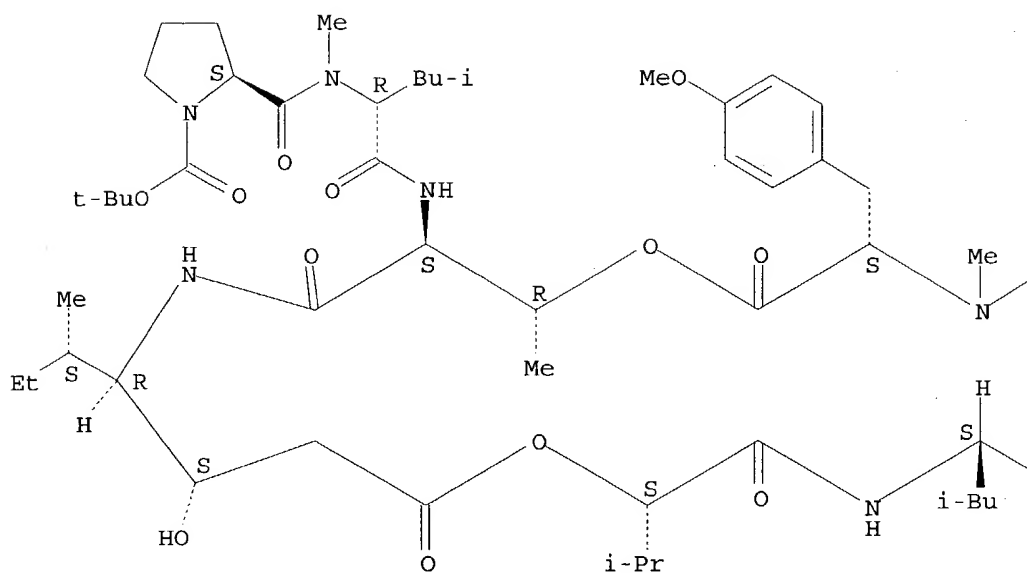


RN 387823-84-9 HCAPLUS
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 (CA INDEX NAME)

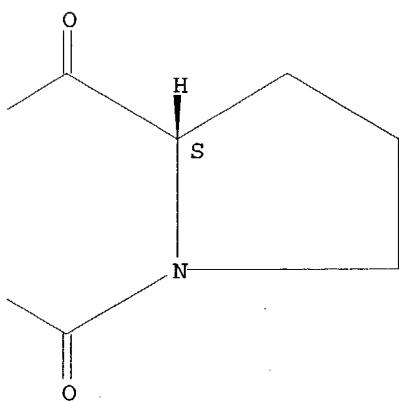
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



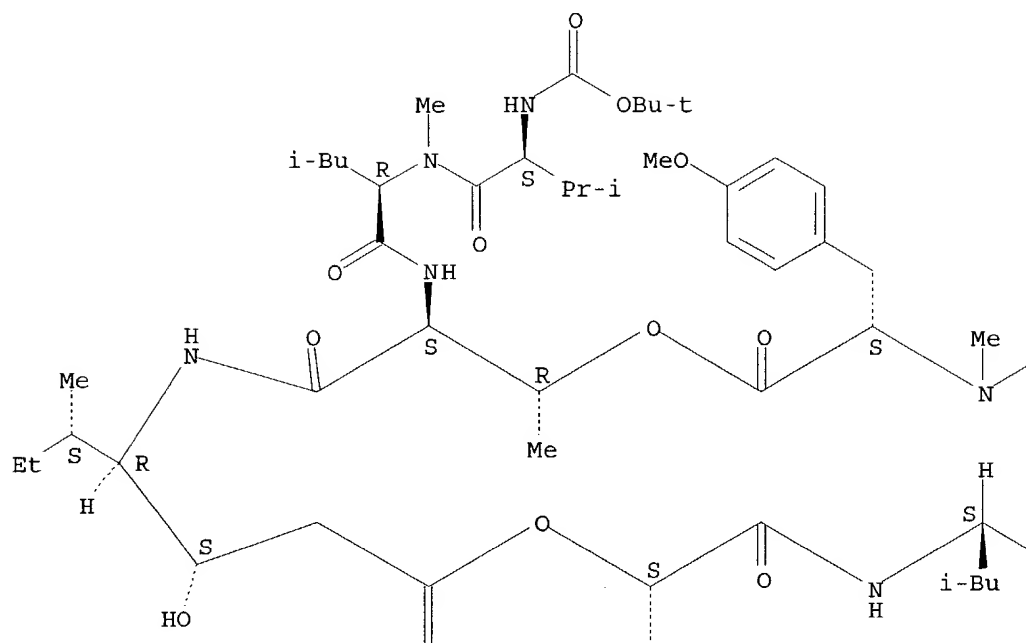
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(CA INDEX NAME)

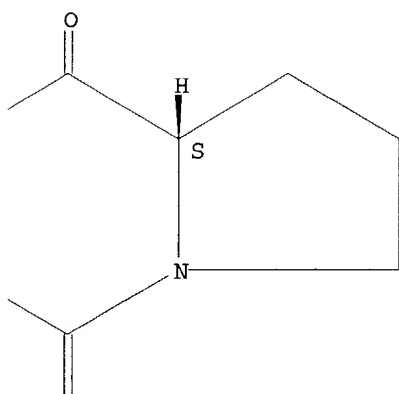
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



PAGE 2-A



PAGE 2-B

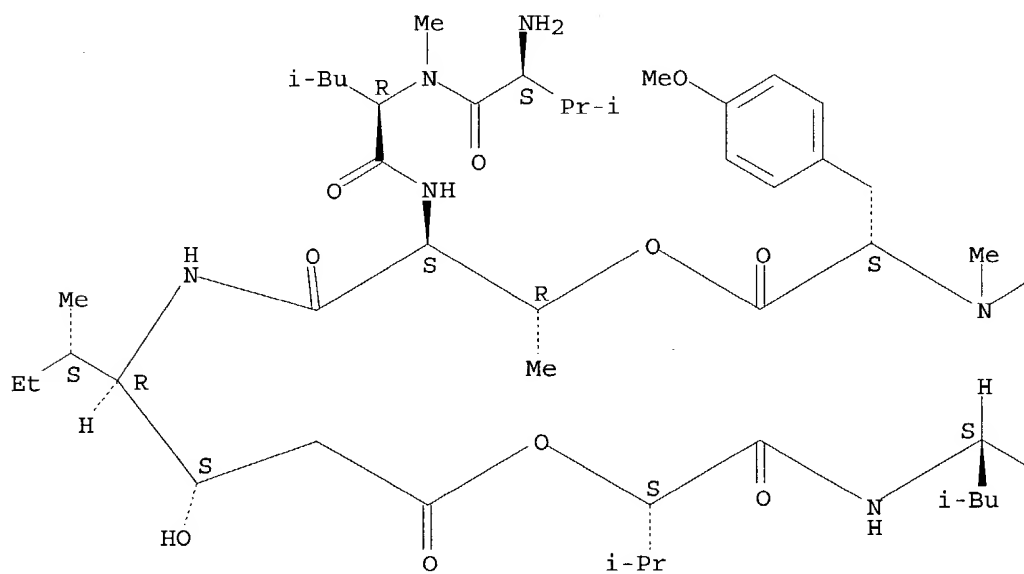


RN 387823-86-1 HCAPLUS

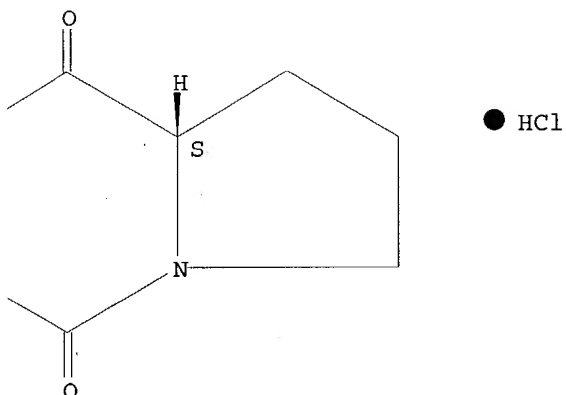
CN L-Tyrosine, L-valyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



IT 345969-81-5P 367507-67-3P 387823-47-4P
 387823-48-5P 387823-49-6P 387823-50-9P
 387823-52-1P 387823-53-2P 387823-58-7P
 387823-60-1P 387823-75-8P 387823-77-0P
 387823-79-2P 387823-80-5P 387823-81-6P
 387823-83-8P 387823-87-2P 387859-52-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

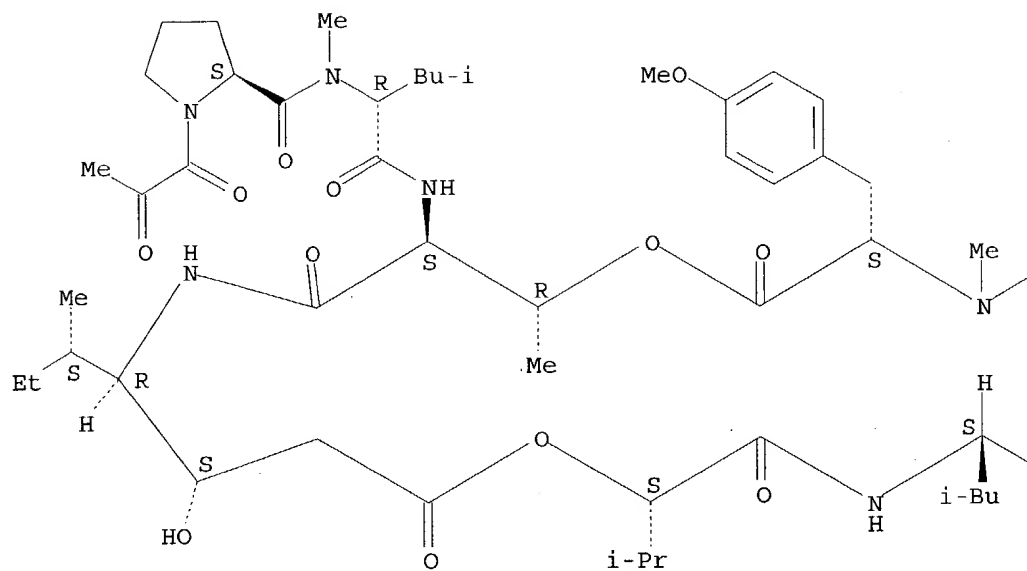
(preparation of aplidine analogs as antitumor agents)

RN 345969-81-5 HCAPLUS

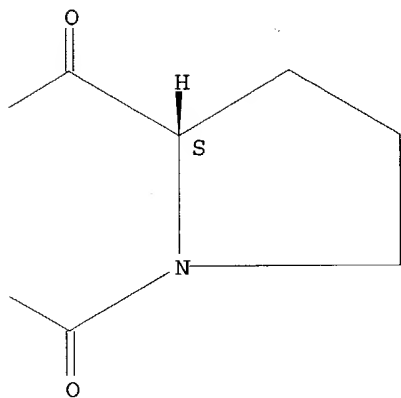
CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B

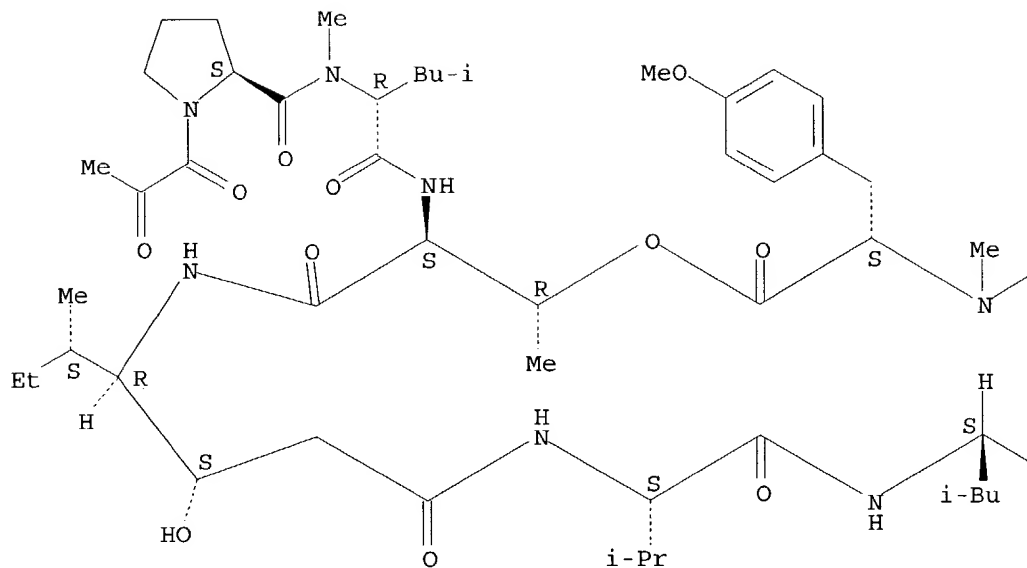


RN 367507-67-3 HCAPLUS
 CN 2-9-Tamandarin A, 2-[1-(1,2-dioxopropyl)-L-proline]-6-L-valine- (9CI) (CA
 INDEX NAME)

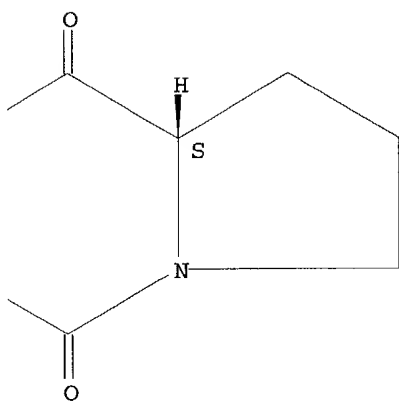
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B

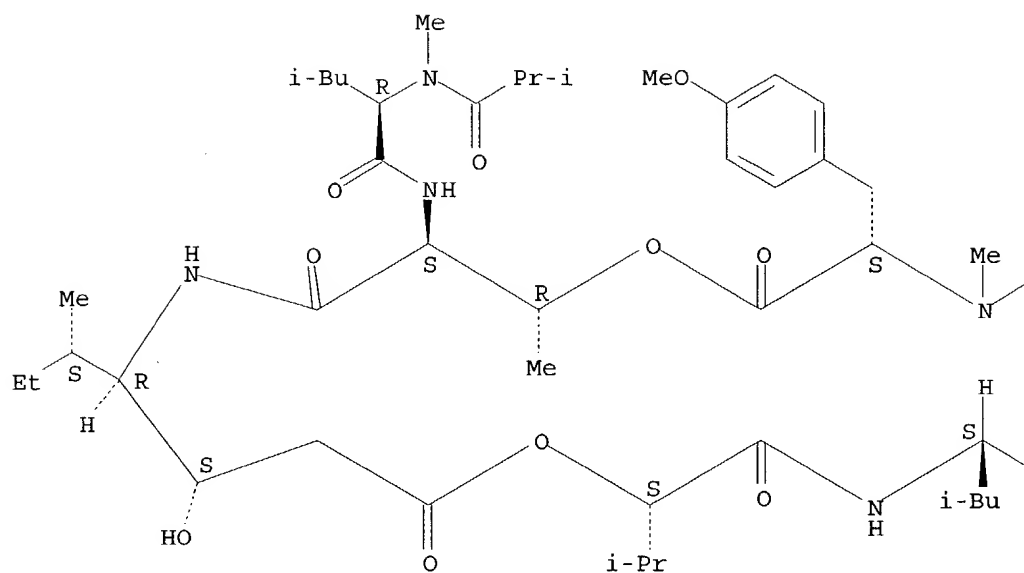


RN 387823-47-4 HCAPLUS
 CN L-Tyrosine, N-methyl-N-(2-methyl-1-oxopropyl)-D-leucyl-L-threonyl-
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI)
 (CA INDEX NAME)

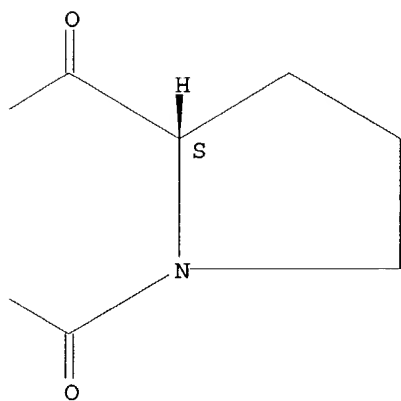
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



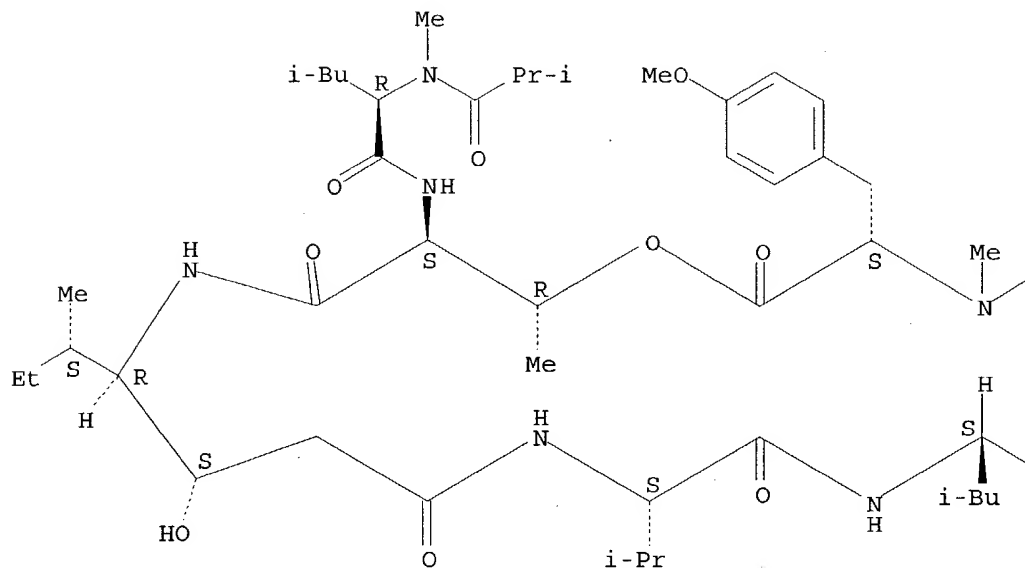
RN 387823-48-5 HCAPLUS

CN L-Tyrosine, N-methyl-N-(2-methyl-1-oxopropyl)-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

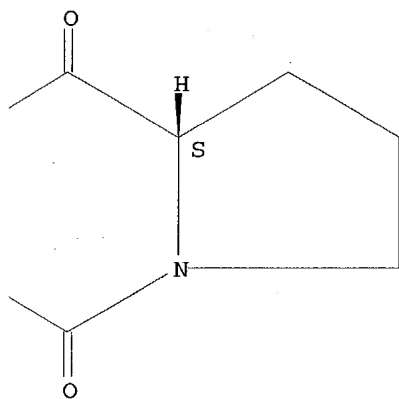
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



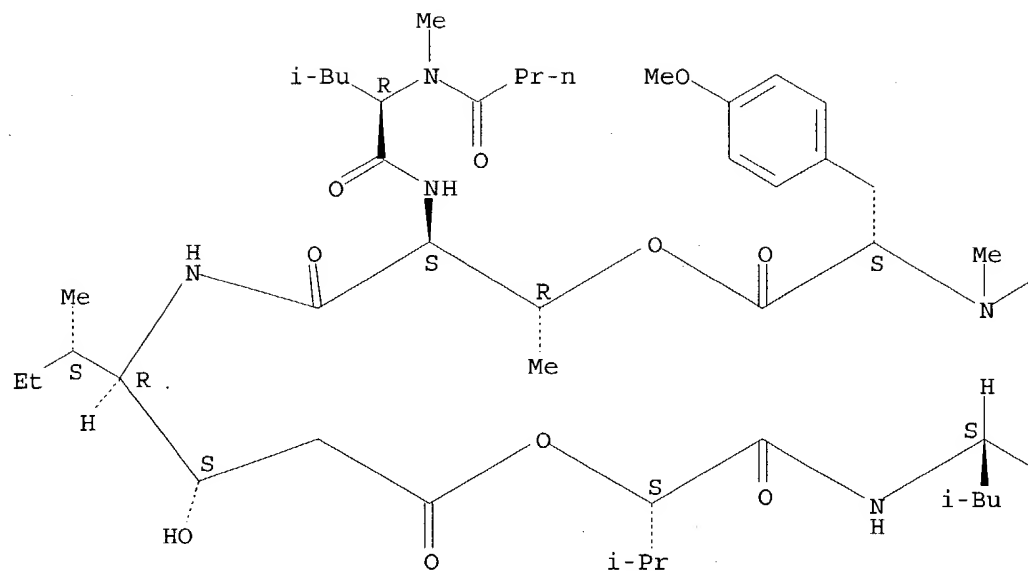
RN 387823-49-6 HCAPLUS

CN L-Tyrosine, N-methyl-N-(1-oxobutyl)-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

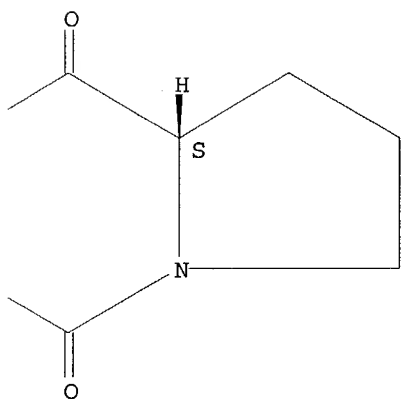
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



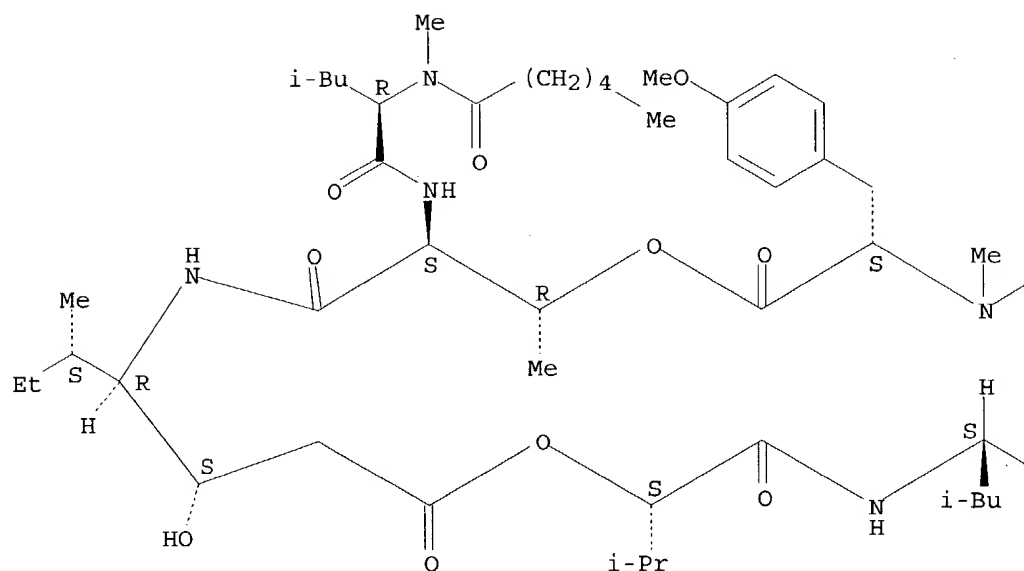
RN 387823-50-9 HCAPLUS

CN L-Tyrosine, N-methyl-N-(1-oxohexyl)-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (7→2)-lactone (9CI) (CA INDEX NAME)

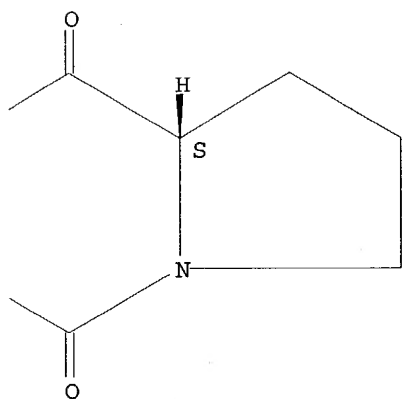
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B

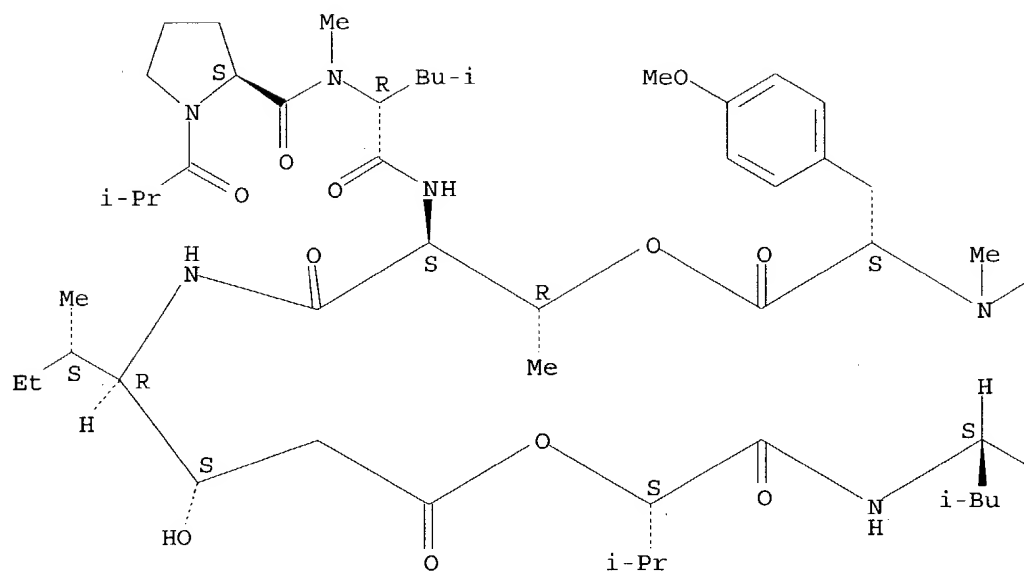


RN	387823-52-1	HCAPLUS
CN	L-Tyrosine, 1-(2-methyl-1-oxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)	
	(CA INDEX NAME)	

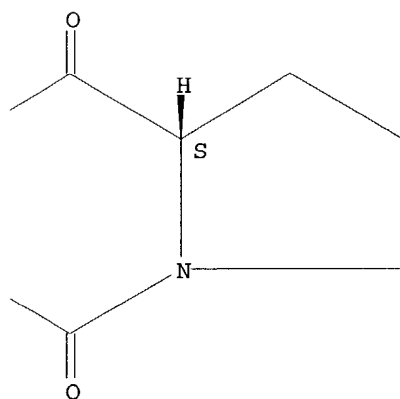
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



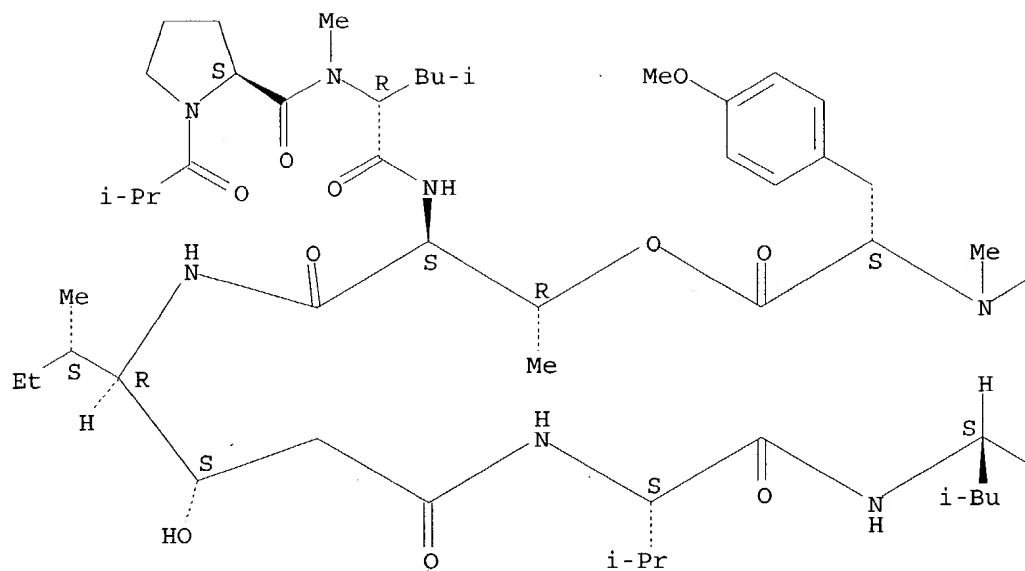
RN 387823-53-2 HCAPLUS

L-Tyrosine, 1-(2-methyl-1-oxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-
 N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

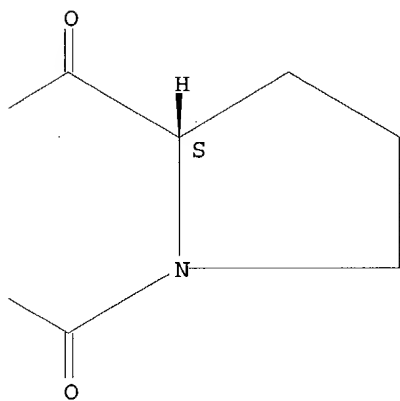
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



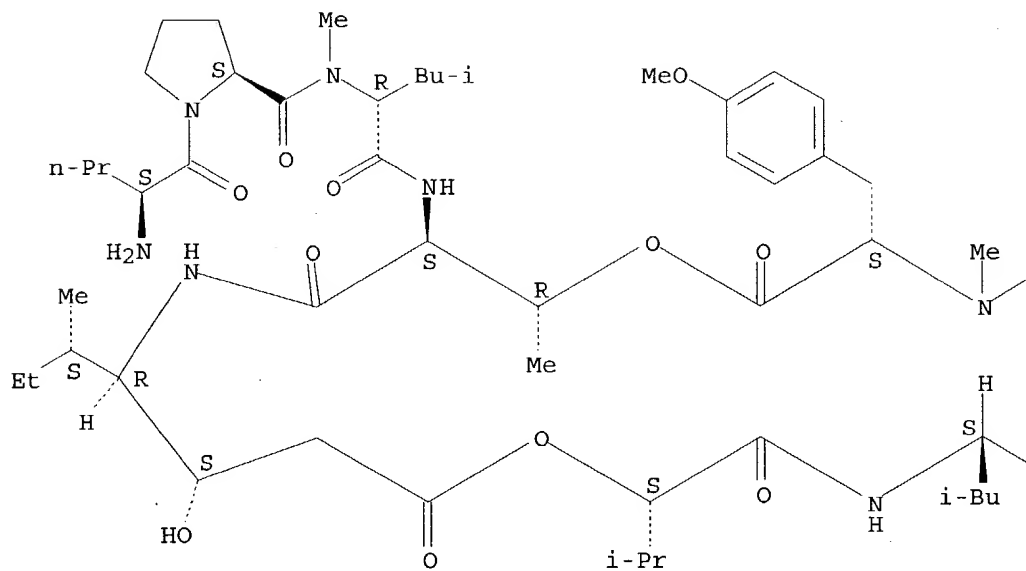
RN 387823-58-7 HCAPLUS

CN L-Tyrosine, L-norvalyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

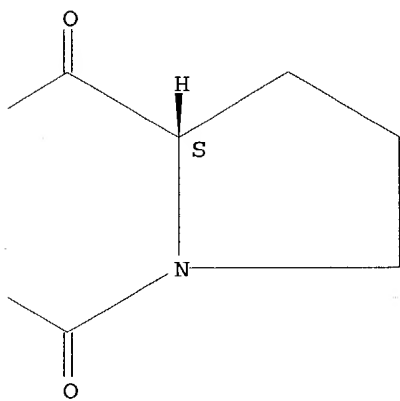
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



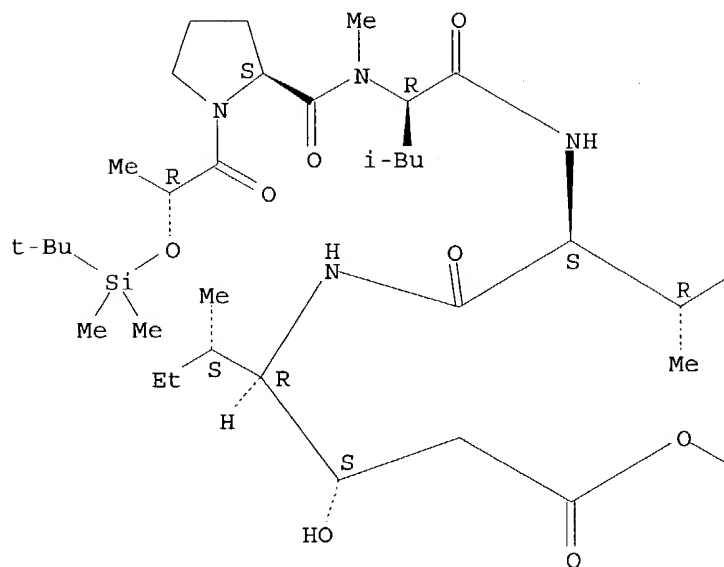
RN 387823-60-1 HCAPLUS

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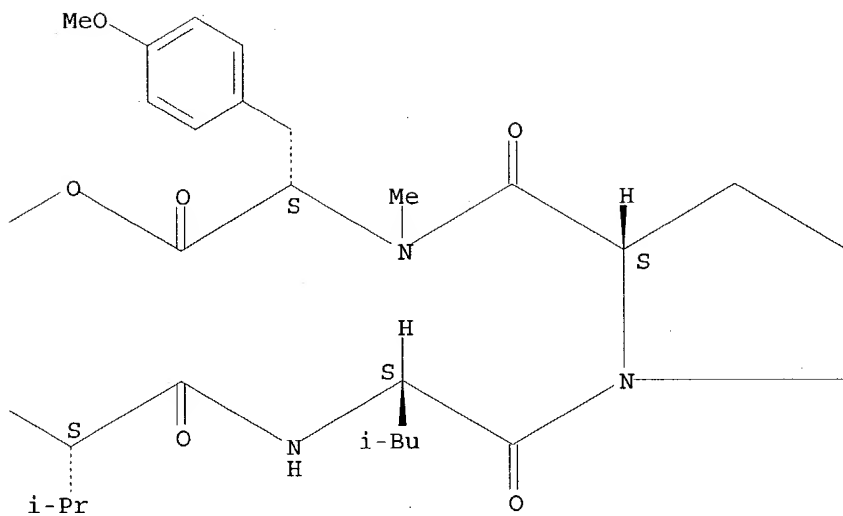
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



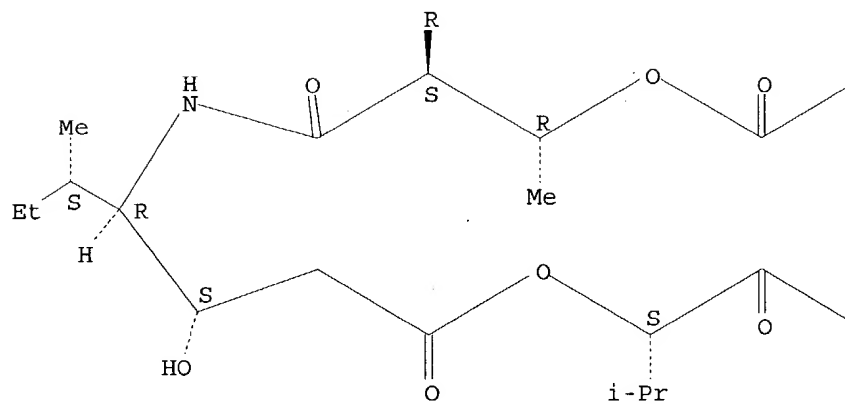
RN 387823-75-8 HCAPLUS

CN L-Tyrosine, N-[(2R)-2-[(5R)-1-[(1,1-dimethylethoxy)carbonyl]-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-4-methyl-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

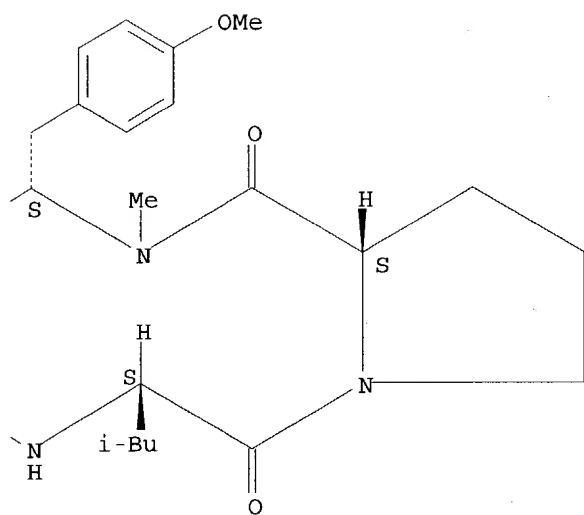
Absolute stereochemistry.

Searched by P. Ruppel

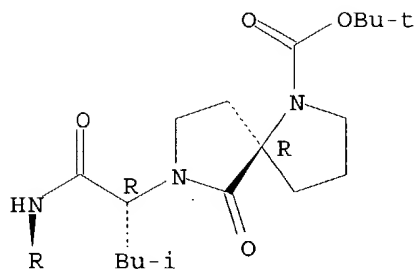
PAGE 1-A



PAGE 1-B



PAGE 2-A

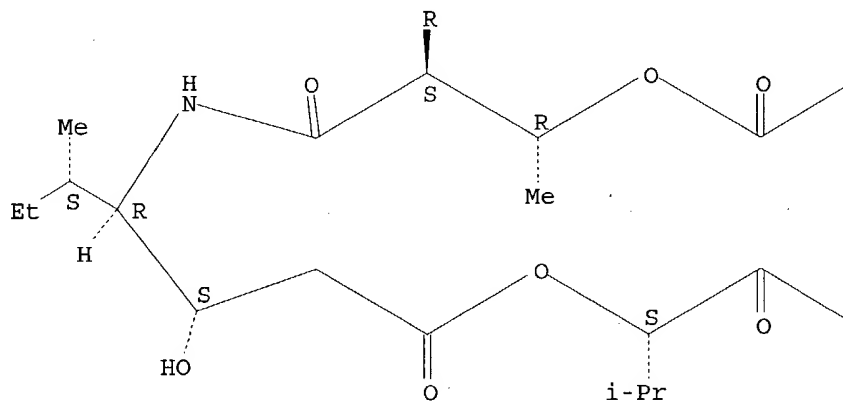


RN 387823-77-0 HCAPLUS

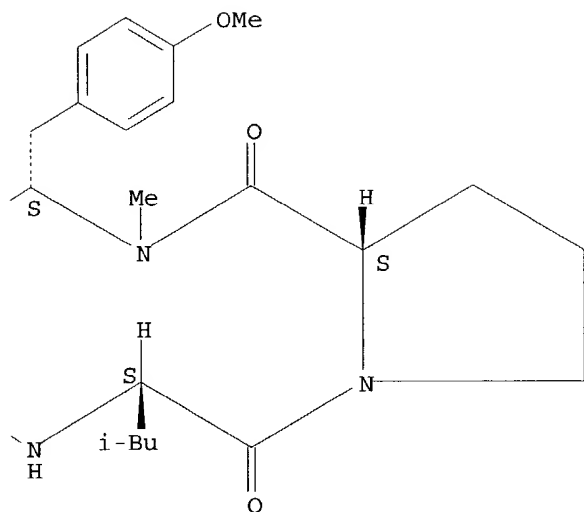
CN L-Tyrosine, N-[(2R)-4-methyl-2-[(5R)-1-(2-methyl-1-oxopropyl)-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

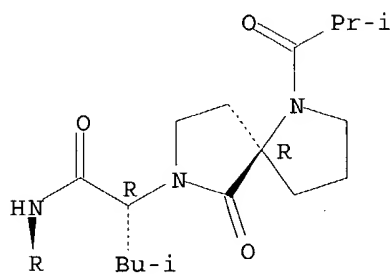
PAGE 1-A



PAGE 1-B



PAGE 2-A

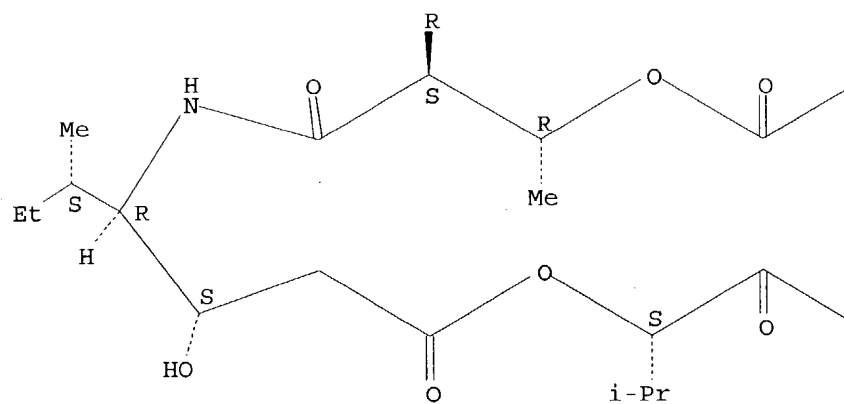


RN 387823-79-2 HCAPLUS

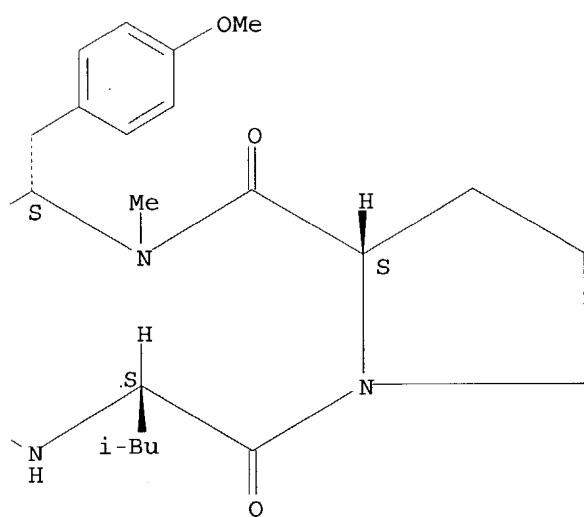
CN L-Tyrosine, N-[(2R)-2-[(5R)-1-(1,2-dioxopropyl)-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-4-methyl-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

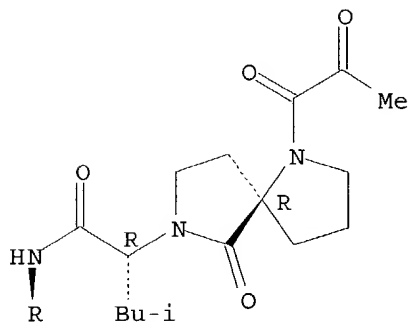
PAGE 1-A



PAGE 1-B



PAGE 2-A

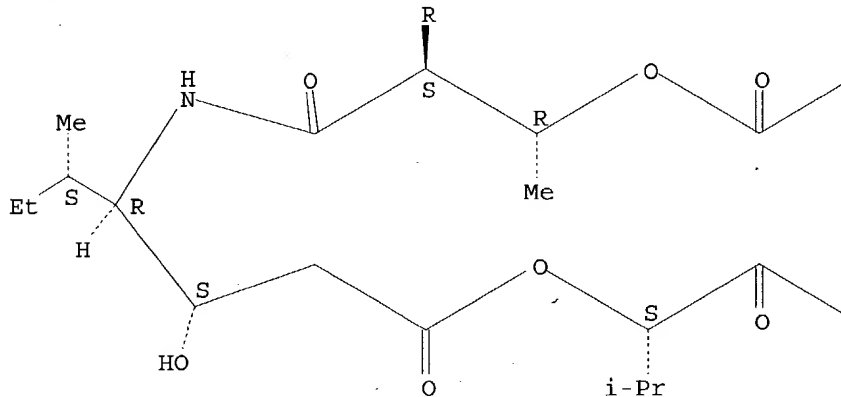


RN 387823-80-5 HCAPLUS

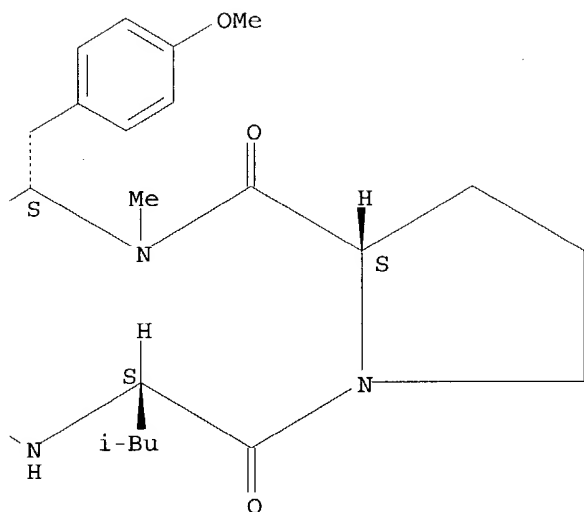
CN L-Tyrosine, N-[(2R)-4-methyl-2-[(5R)-1-(2-methyl-1-oxo-2-propenyl)-6-oxo-1,7-diazaspiro[4.4]non-7-yl]-1-oxopentyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

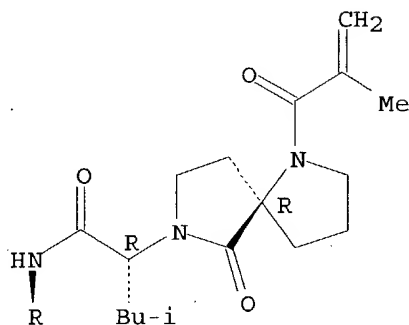
PAGE 1-A



PAGE 1-B



PAGE 2-A

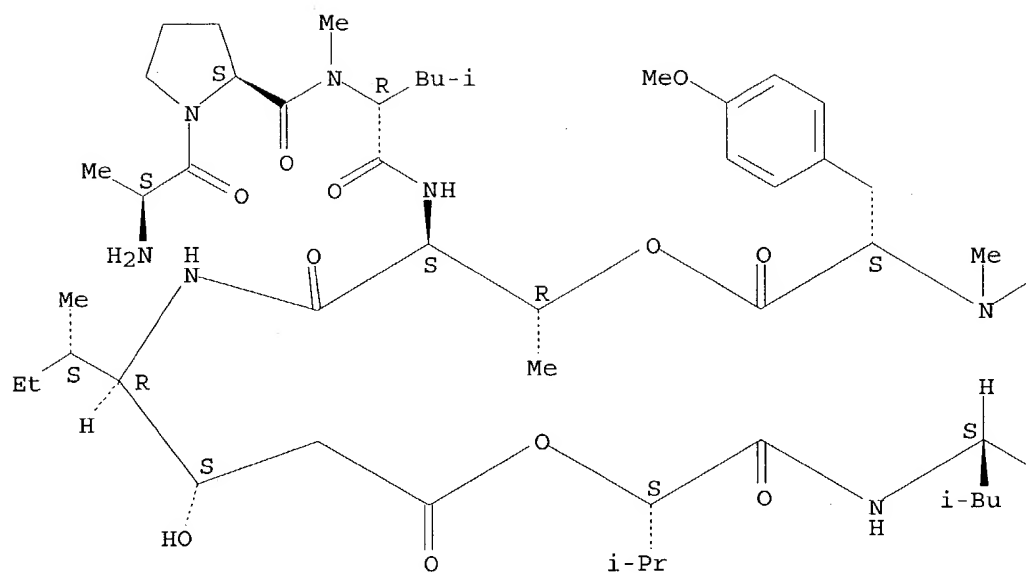


RN 387823-81-6 HCAPLUS

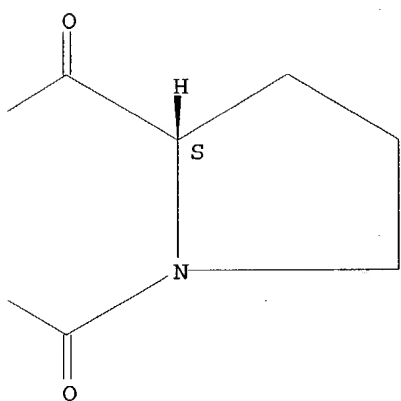
CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



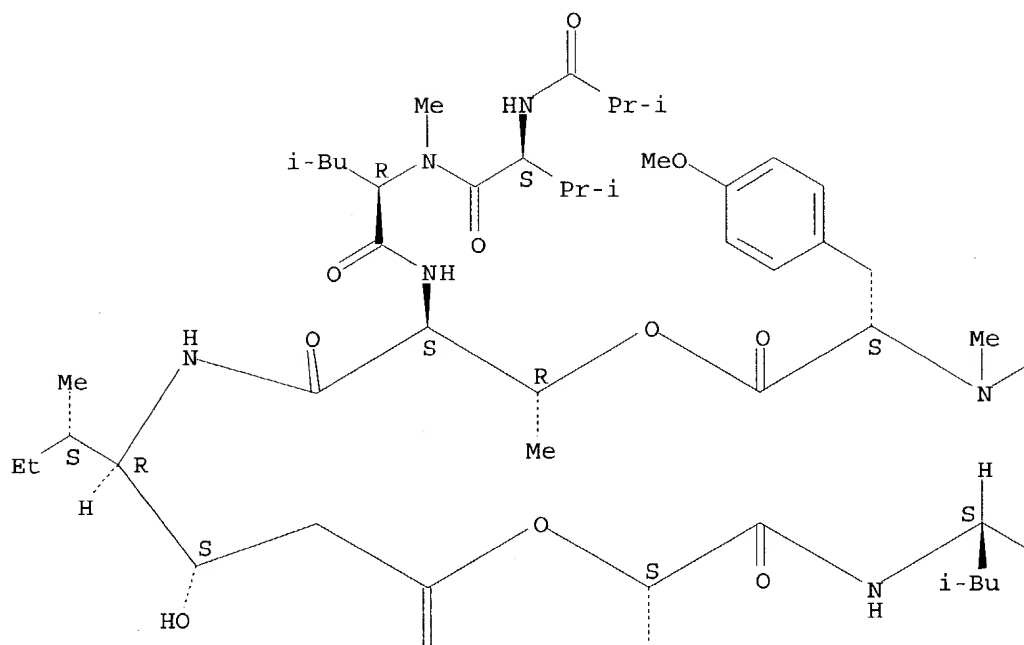
● HCl

RN 387823-87-2 HCAPLUS
 CN L-Tyrosine, N-(2-methyl-1-oxopropyl)-L-valyl-N-methyl-D-leucyl-L-threonyl-
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)
 (CA INDEX NAME)

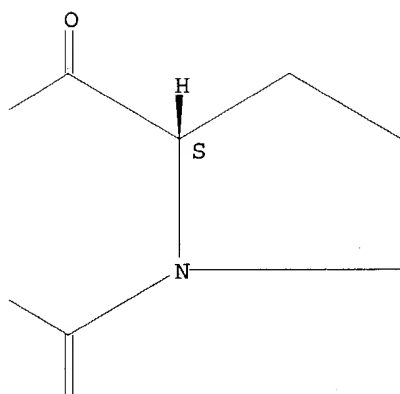
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



PAGE 2-A



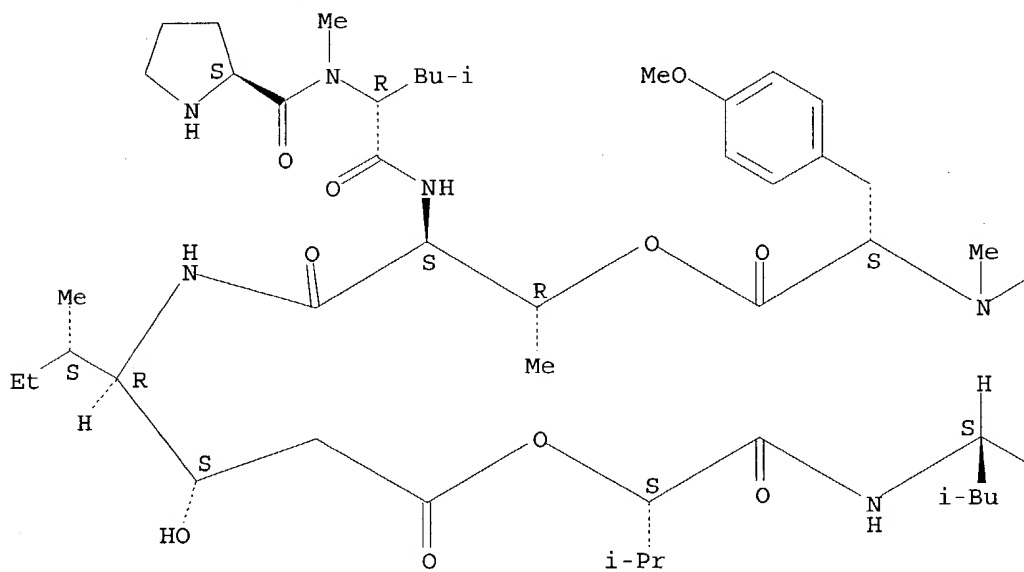
PAGE 2-B



RN 387859-52-1 HCAPLUS
 CN L-Tyrosine, L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

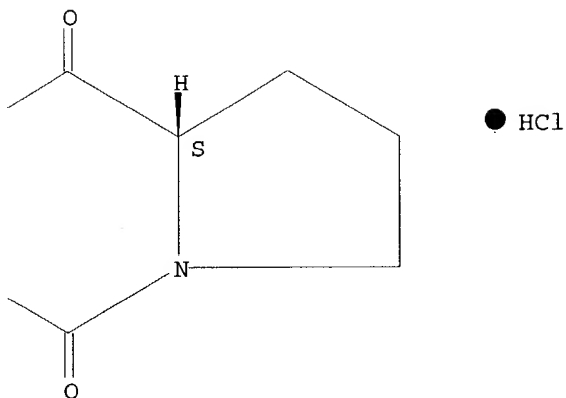
Absolute stereochemistry. Rotation (-).

PAGE 1-A



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PAGE 1-B



IT 291772-83-3P 387823-38-3P 387823-39-4P
387823-41-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

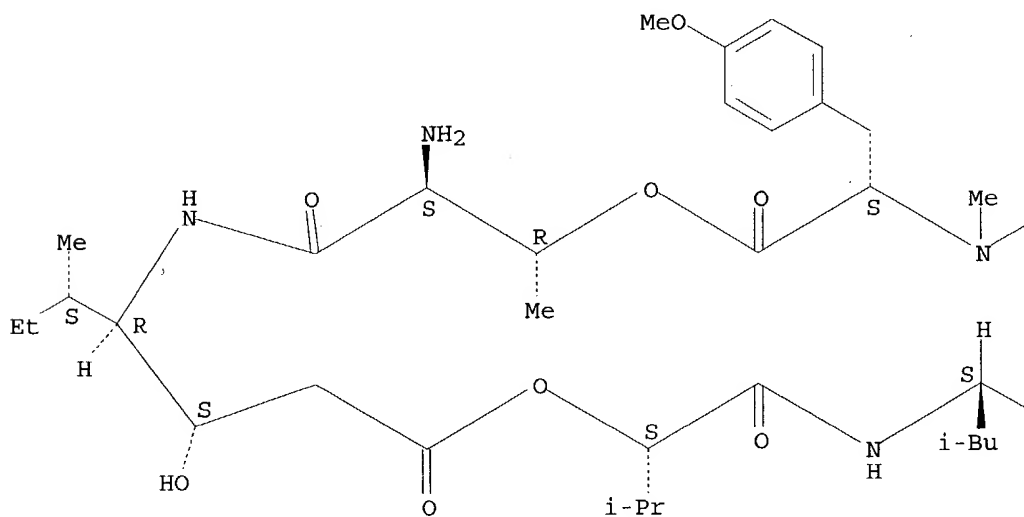
(preparation of aplidine analogs as antitumor agents)

RN 291772-83-3 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-
2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-,
(6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

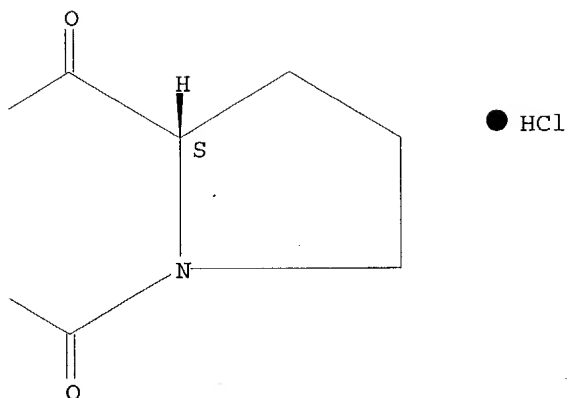
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

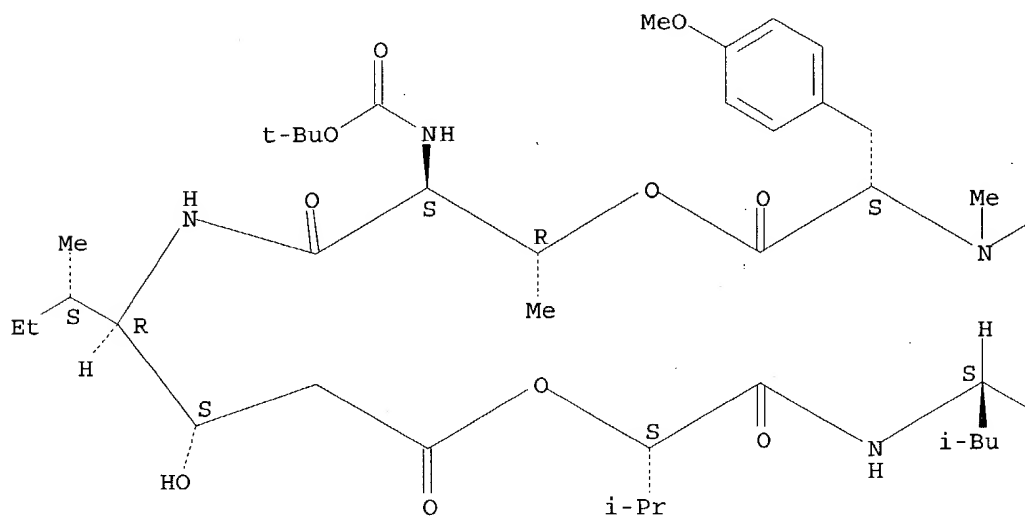


RN 387823-38-3 HCAPLUS

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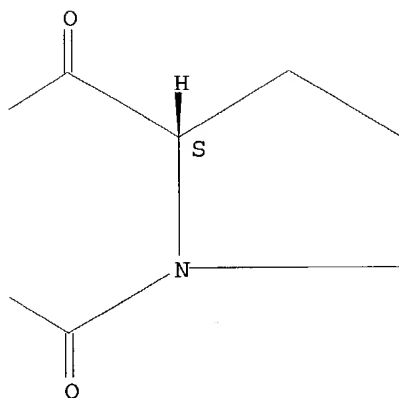
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

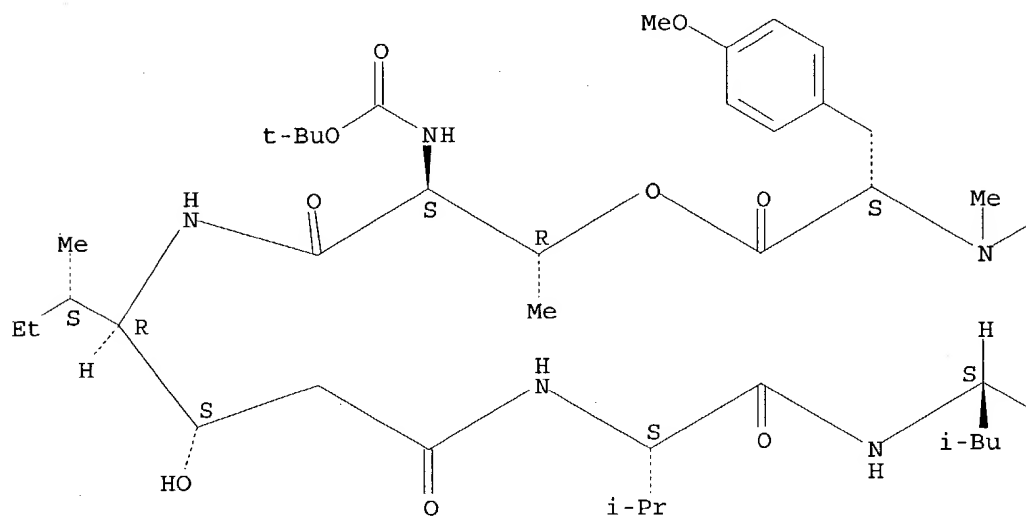


RN 387823-39-4 HCAPLUS

CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI) (CA INDEX NAME)

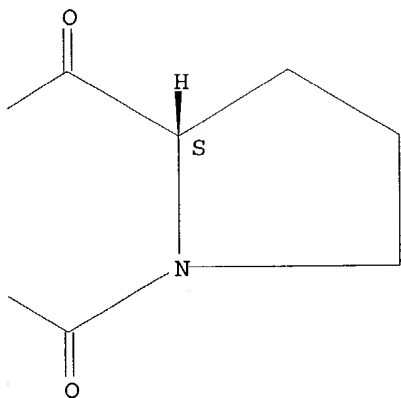
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

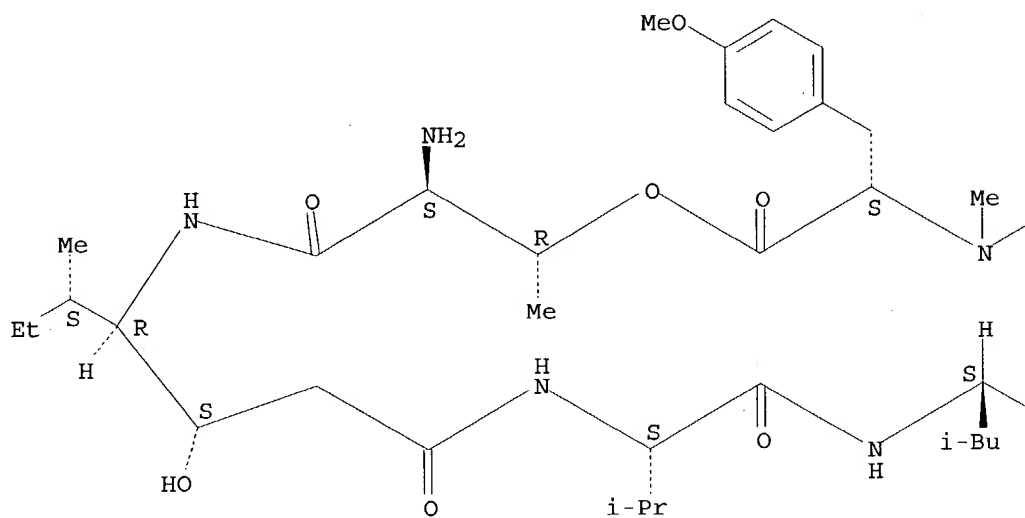


RN 387823-41-8 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-L-valyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

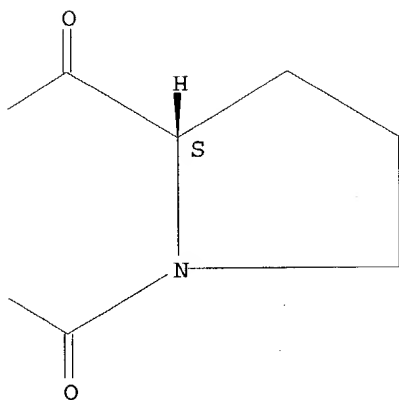
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

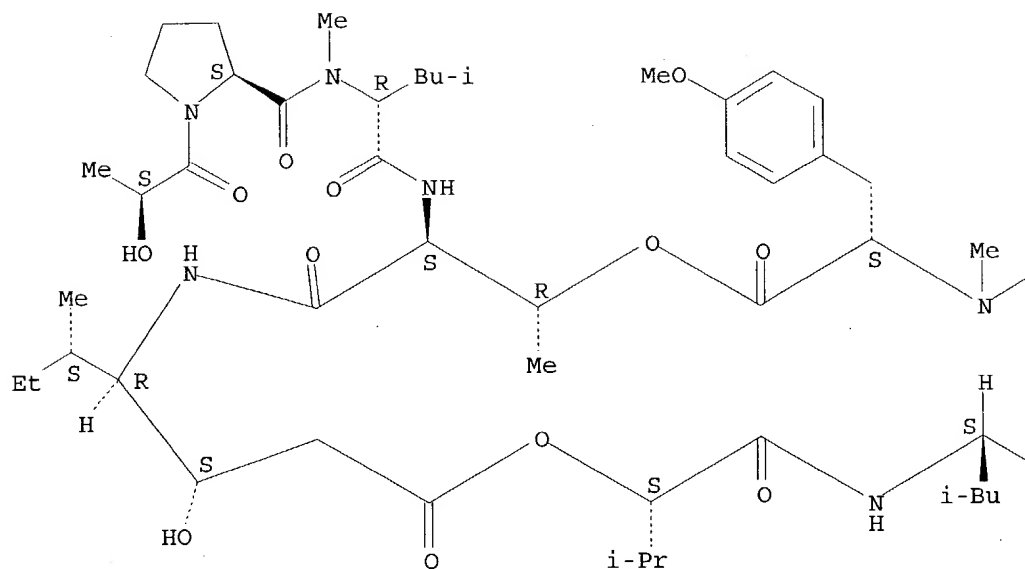


● HCl

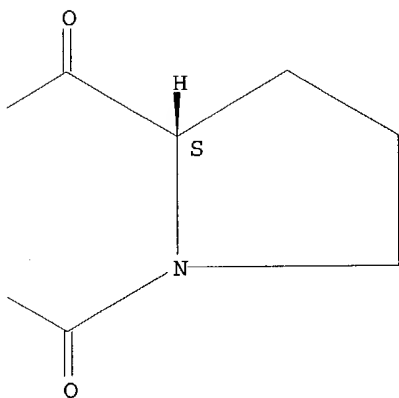
L62 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:16567 HCAPLUS
DOCUMENT NUMBER: 137:140752
TITLE: Part I. Total synthesis and biological investigations
of tamandarin compounds. Part II. Synthetic studies
towards the total synthesis of callipeltin A
AUTHOR(S): Liang, Bo
CORPORATE SOURCE: Univ. of Pennsylvania, Philadelphia, PA, USA
SOURCE: (2001) 455 pp. Avail.: UMI, Order No. DA3003653
From: Diss. Abstr. Int., B 2001, 62(2), 864
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 250211-78-0P, Tamandarin A
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(total synthesis and biol. investigations of tamandarin compds.)
RN 250211-78-0 HCAPLUS
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



L62 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:762837 HCAPLUS
DOCUMENT NUMBER: 135:318713
TITLE: Preparation of tamandarin and didemnin analogs
INVENTOR(S): Jöullie, Madeleine M.; Liang, Bo; Ding, Xiaobin
PATENT ASSIGNEE(S): Trustees of the University of Pennsylvania, USA
SOURCE: PCT Int. Appl., 190 pp.

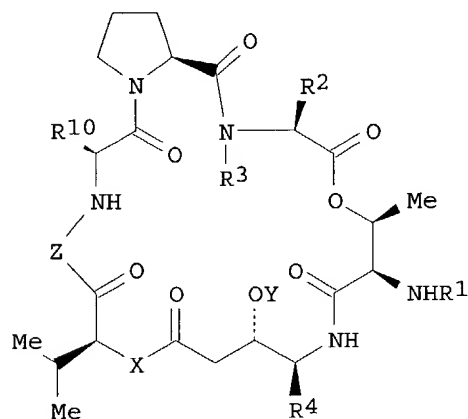
Searched by P. Ruppel

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001076616	A1	20011018	WO 2001-US11607	20010409
W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	
RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	
US 6509315	B1	20030121	US 2000-545848	20000407
US 2001056178	A1	20011227	US 2001-767080	20010122
EP 1276491	A1	20030122	EP 2001-924886	20010409
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR	
BR 2001009958	A	20030527	BR 2001-9958	20010409
JP 2003535048	T2	20031125	JP 2001-574132	20010409
PRIORITY APPLN. INFO.:			US 2000-545848 A	20000407
			US 2001-767080 A	20010122
			WO 2001-US11607 W	20010409

OTHER SOURCE(S): CASREACT 135:318713; MARPAT 135:318713

GI



I

AB The invention relates to tamandarin and didemnin analogs I (Z = null or COCHMe, resp.; R1 = H, tert-butoxycarbonyl, leucyl, N-methyllleucyl, a residue having a deoxoproline or dehydroproline residue, etc.; R2 is an isoleucine, valine, alanine, norleucine, norvaline, leucine, histidine, tryptophan, arginine or lysine side chain or a substituted benzyl group; R3 = H, Me or R2R3 is a substituted o-phenylenemethylene group; R4 is an isoleucine or valine side chain; X = O or NH; Y = H or a hydroxy-protecting group) which are useful as anticancer agents, inhibitors of protein synthesis, cell growth and tumorigenesis and as enhancers of apoptosis. (-)-Tamandarin A is not claimed but a total

synthesis was carried out. The synthesis of a didemnin B analog in which R1 is 3,4-dehydro-L-prolyl-N-methyl-D-leucyl is described.

IT 250211-78-0P, Tamandarin a 258339-38-7P, Tamandarin B

291772-81-1P, Tamandarin M 345969-81-5P

367507-41-3P 367507-42-4P 367507-44-6P

367507-45-7P 367507-46-8P 367507-47-9P

367507-48-0P 367507-49-1P 367507-50-4P

367507-51-5P 367507-52-6P 367507-53-7P

367507-54-8P 367507-55-9P 367507-56-0P

367507-57-1P 367507-58-2P 367507-59-3P

367507-60-6P 367507-61-7P 367507-62-8P

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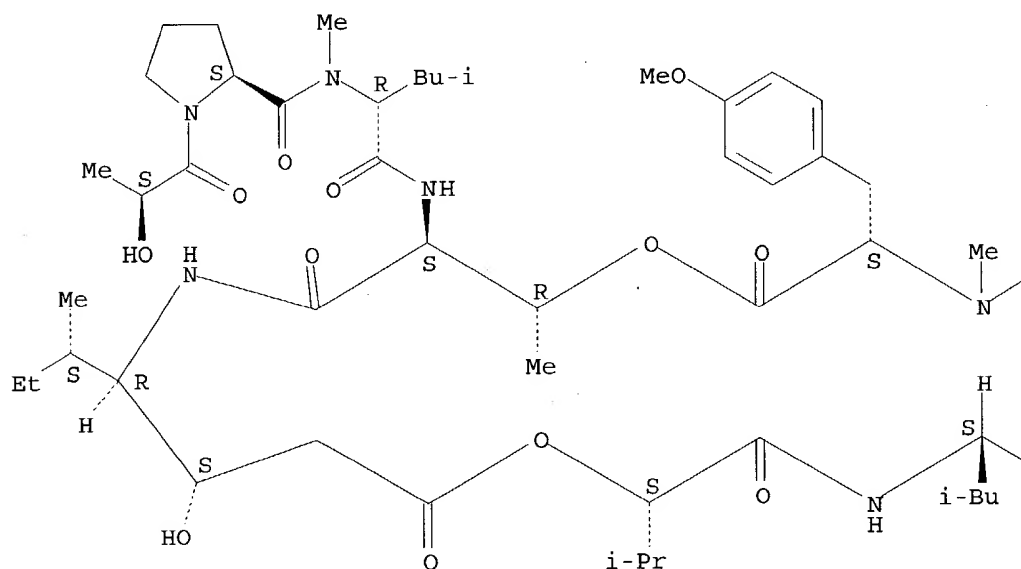
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tamandarin and didemnin analogs)

RN 250211-78-0 HCAPLUS

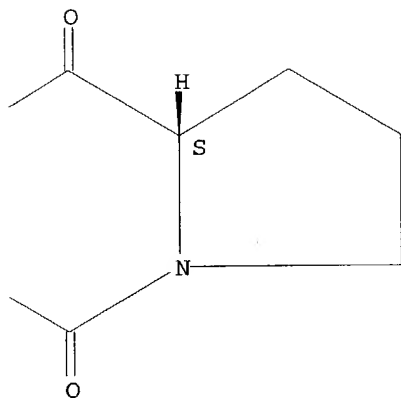
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



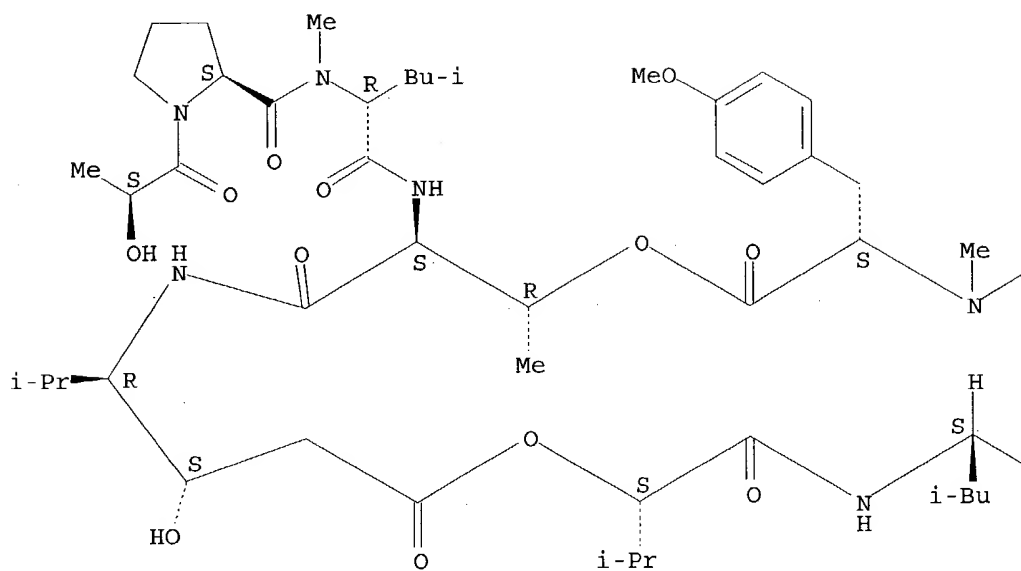
PAGE 1-B



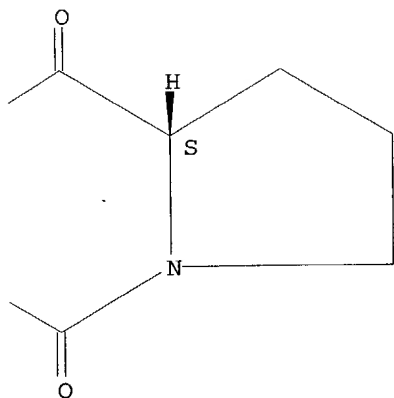
RN 258339-38-7 HCAPLUS
CN Tamandarin B (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



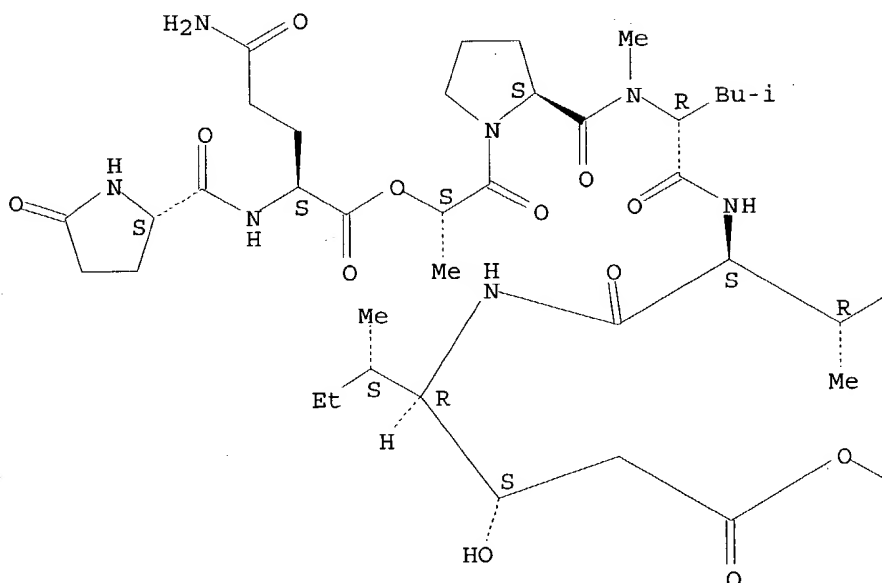
PAGE 1-B



RN 291772-81-1 HCAPLUS
CN Didemnin M, 8-[(2S)-2-hydroxy-3-methylbutanoic acid]- (9CI) (CA INDEX
NAME)

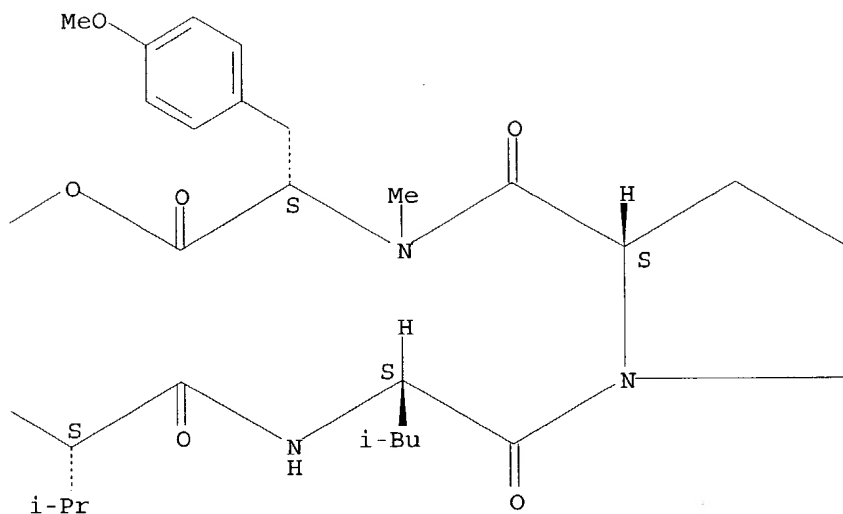
Absolute stereochemistry. Rotation (-).

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

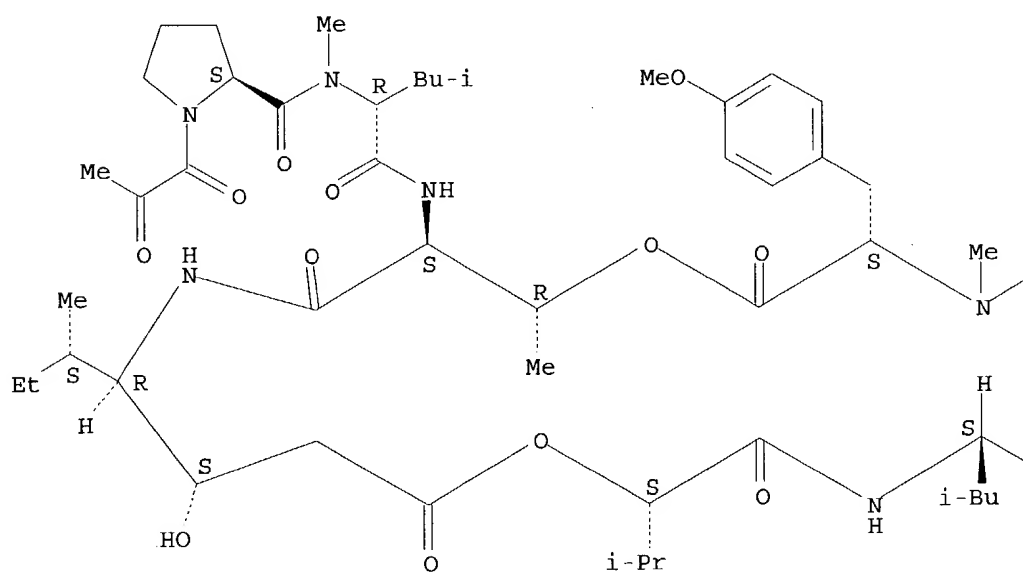


RN 345969-81-5 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-
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 (CA INDEX NAME)

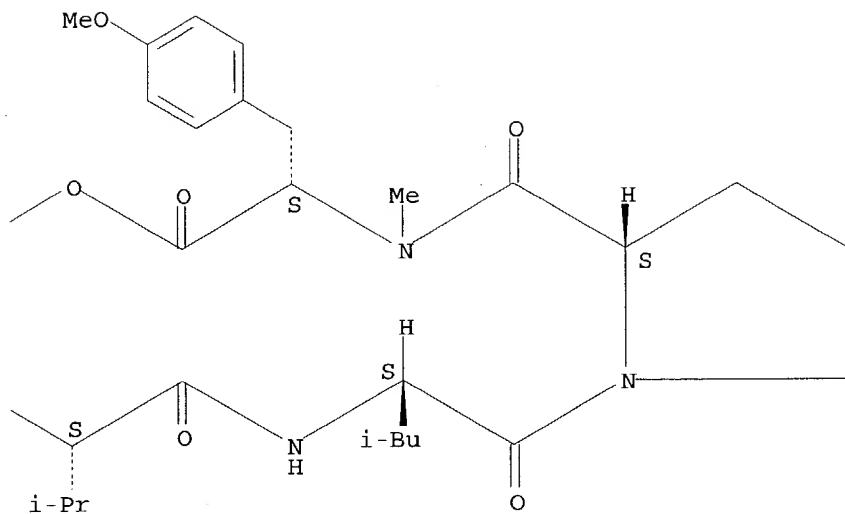
Absolute stereochemistry. Rotation (-).

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

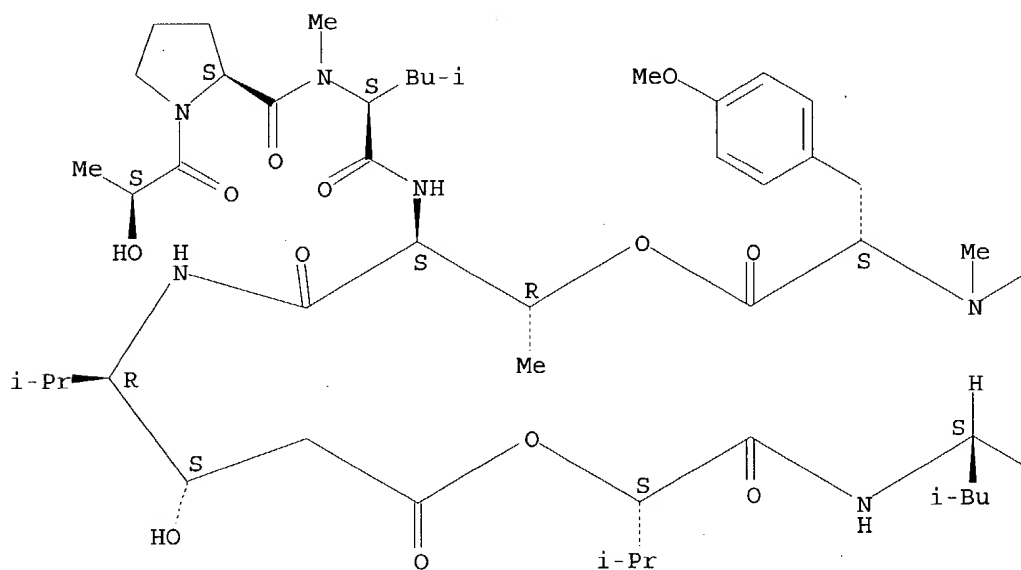


RN 367507-42-4 HCAPLUS

CN L-Tyrosine, (2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-L-leucyl-L-threonyl-
 (3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-
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 NAME)

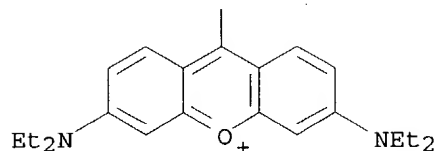
Absolute stereochemistry.

PAGE 1-A



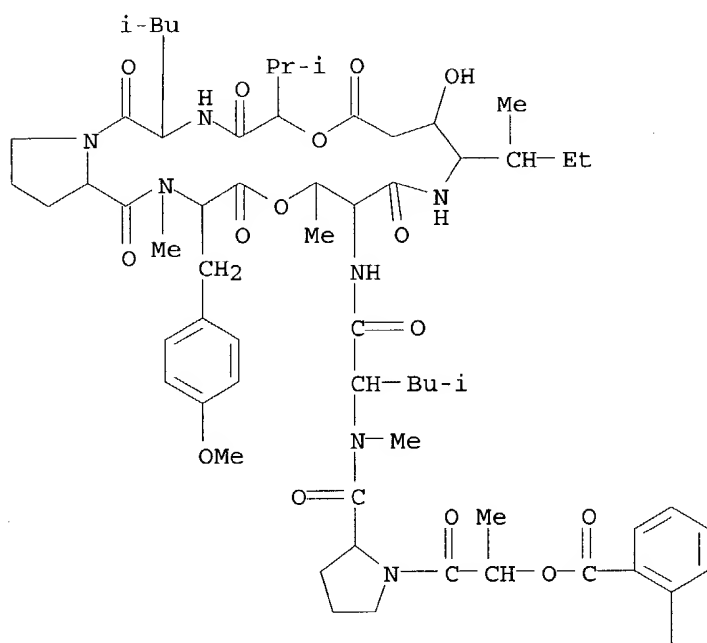
Searched by P. Ruppel

PAGE 2-A

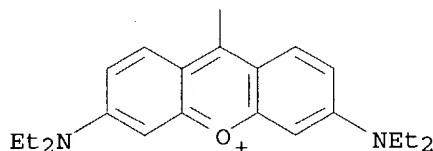


RN 367507-45-7 HCAPLUS
 CN Tamandarin A, 3-(N-methyl-L-leucine)-, 1-[2-[3,6-bis(diethylamino)xanthylum-9-yl]benzoate] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

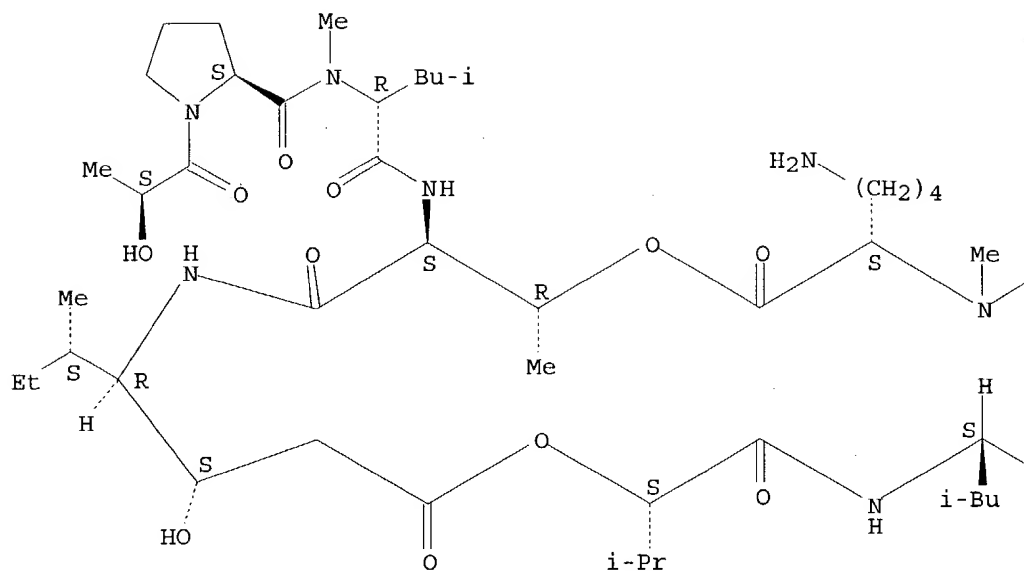


RN 367507-46-8 HCAPLUS
 CN L-Lysine, (2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N2-methyl-, (9→4)-lactone (9CI)
 (CA INDEX NAME)

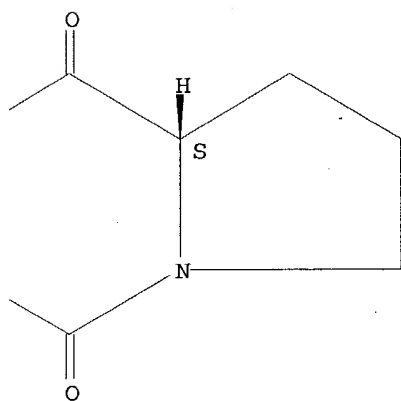
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



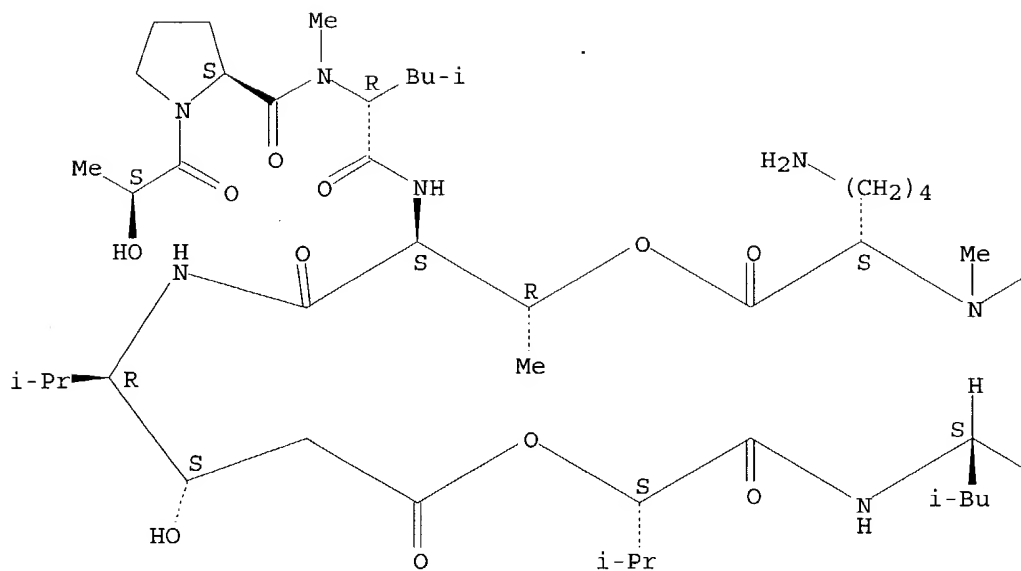
RN 367507-47-9 HCAPLUS

CN L-Lysine, (2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-
(3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-
L-leucyl-L-prolyl-N2-methyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

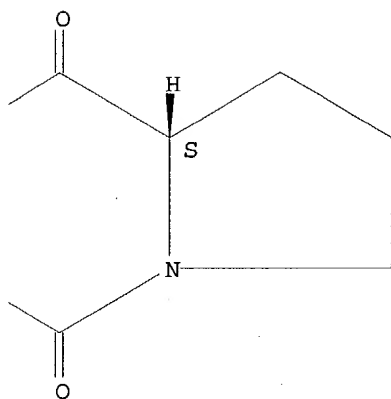
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



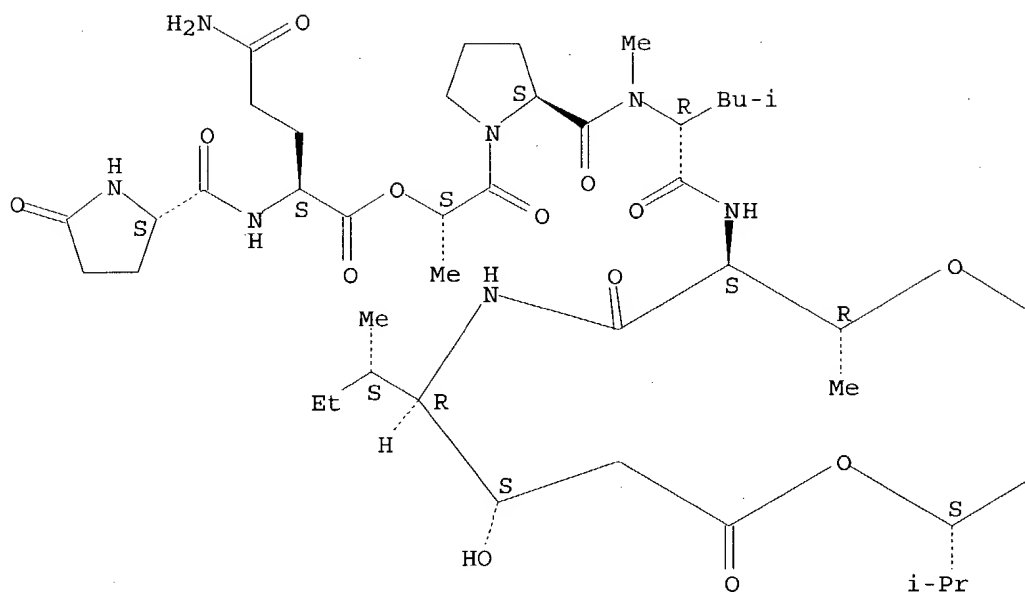
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CN L-Lysine, 5-oxo-L-prolyl-L-glutamyl-(2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N2-methyl-, (11→6)-lactone (9CI) (CA INDEX NAME)

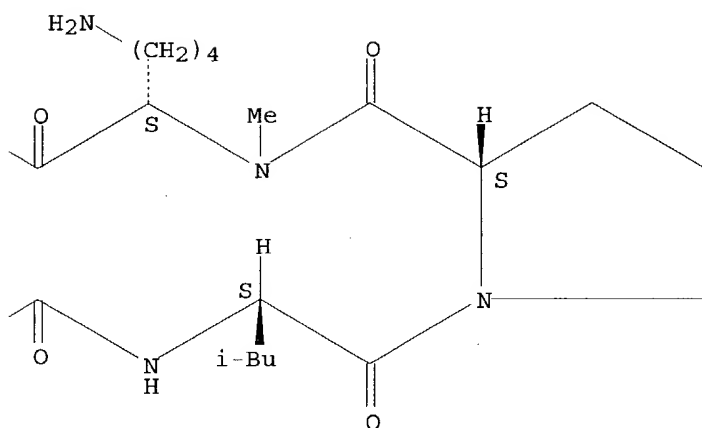
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



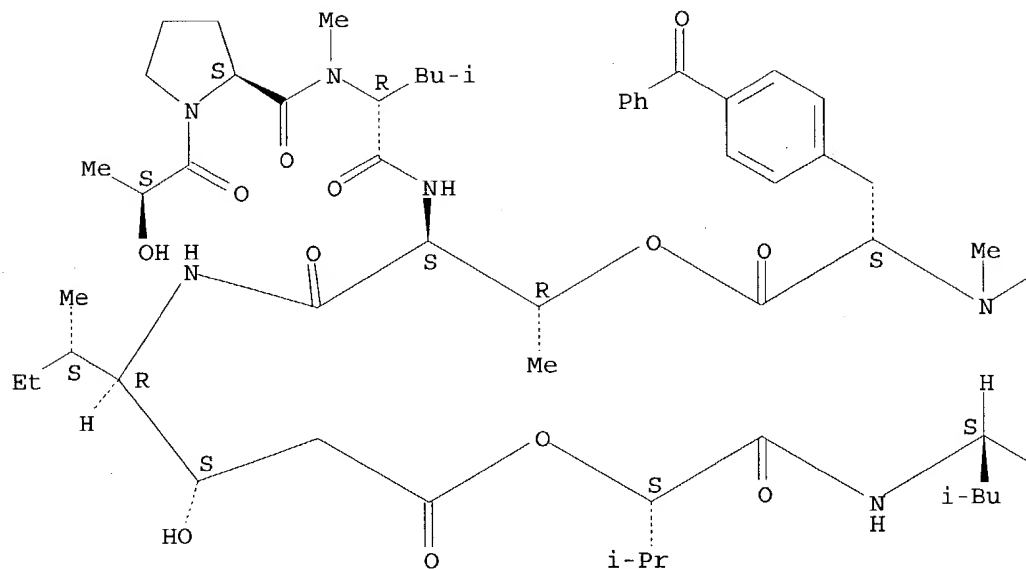
RN 367507-49-1 HCAPLUS

CN L-Phenylalanine, (2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-4-benzoyl-N-methyl-, (9→4)-lactone
(9CI) (CA INDEX NAME)

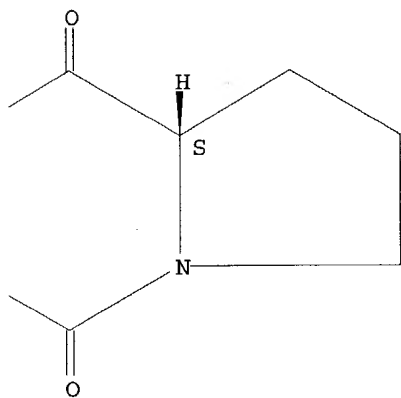
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



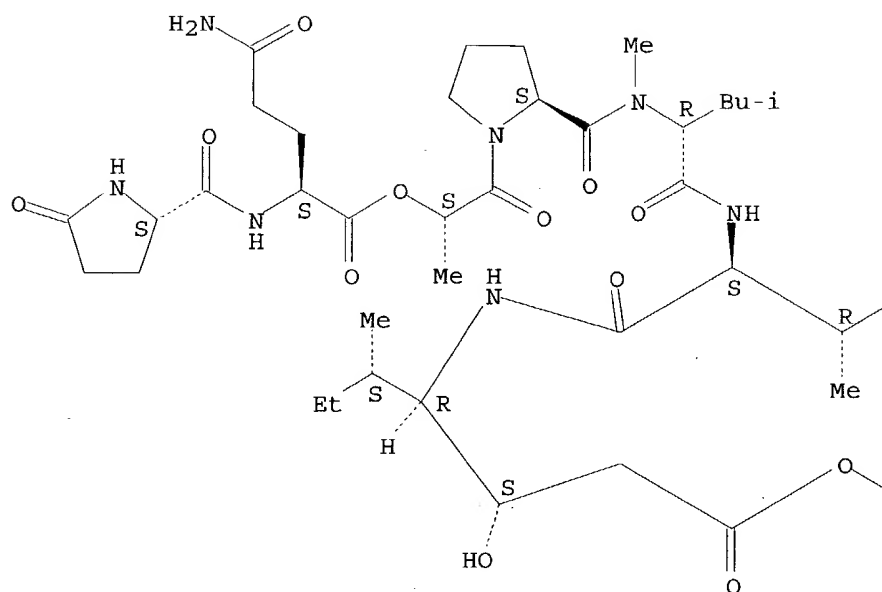
RN 367507-50-4 HCAPLUS

CN L-Phenylalanine, 5-oxo-L-prolyl-L-glutaminyl-(2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-4-benzoyl-N-methyl-, (11→6)-lactone (9CI) (CA INDEX NAME)

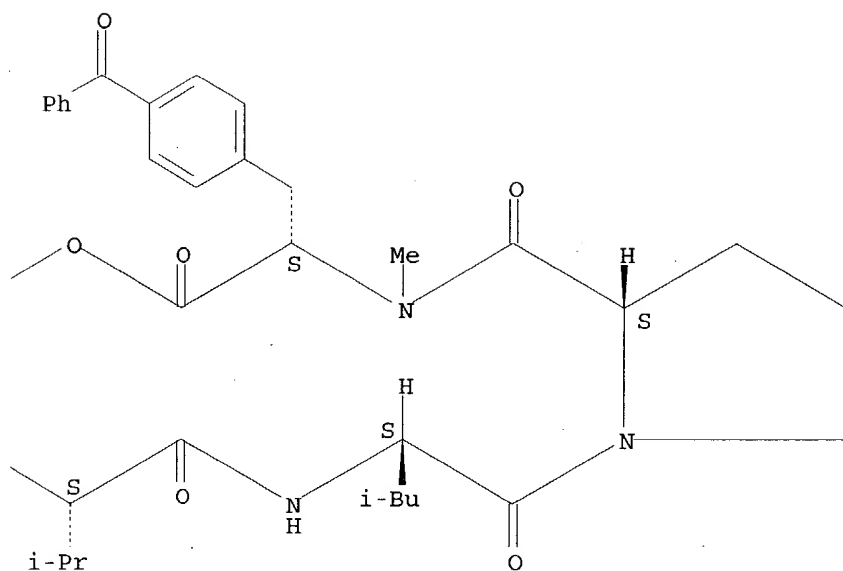
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



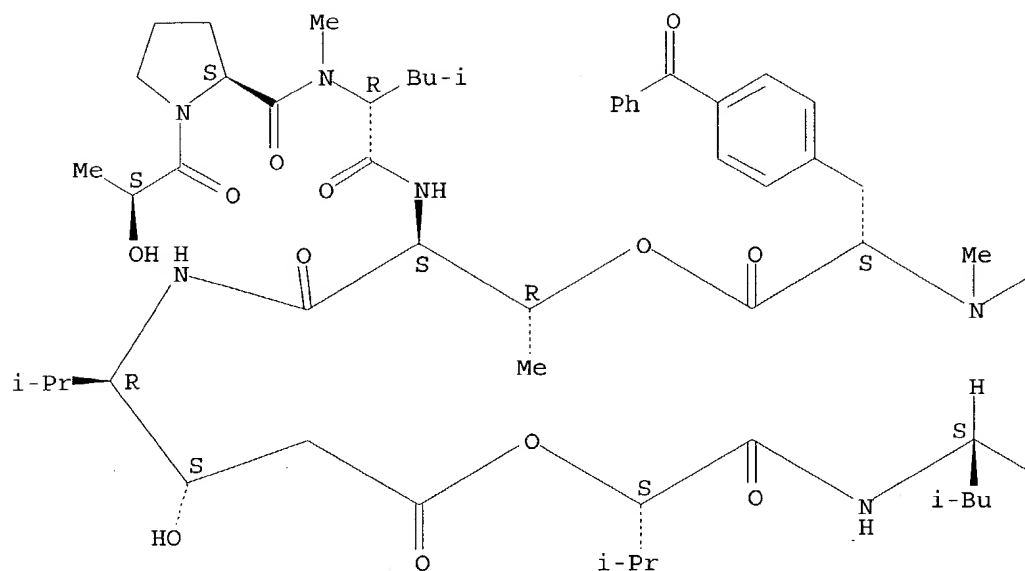
RN 367507-51-5 HCAPLUS

CN L-Phenylalanine, (2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-4-benzoyl-N-methyl-, (9→4)-lactone (9CI) (CA INDEX NAME)

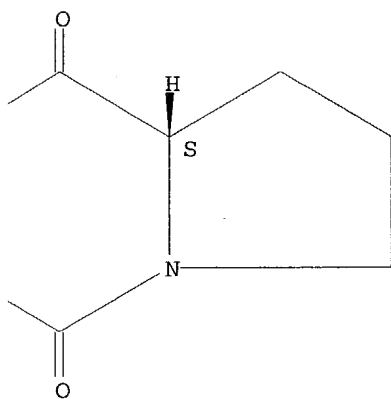
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



RN 367507-52-6 HCAPLUS
 CN Tamandarin A, 9-[(3S)-1,2,3,4-tetrahydro-7-methoxy-3-isoquinolinecarboxylic acid]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 367507-53-7 HCAPLUS
 CN Tamandarin A, 9-[(3S)-1,2,3,4-tetrahydro-7-methoxy-3-isoquinolinecarboxylic acid]-, (2'→1)-ester with

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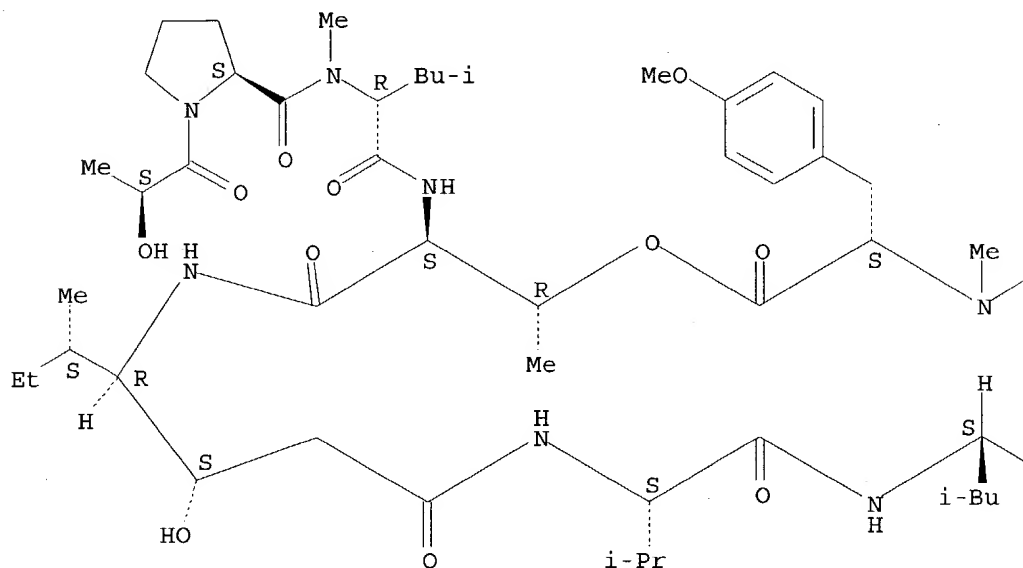
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CN Tamandarin B, 9-[(3S)-1,2,3,4-tetrahydro-7-methoxy-3-isoquinolinecarboxylic acid]-(9CI) (CA INDEX NAME)

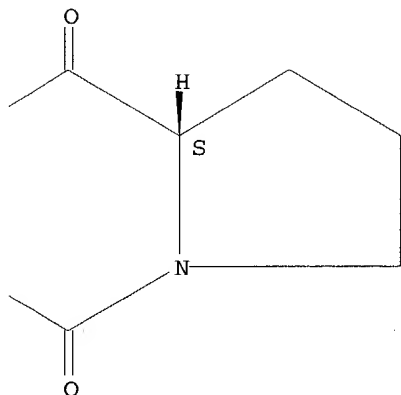
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CN Tamandarin A, 6-L-valine- (9CI) (CA INDEX NAME)

PAGE 1-A



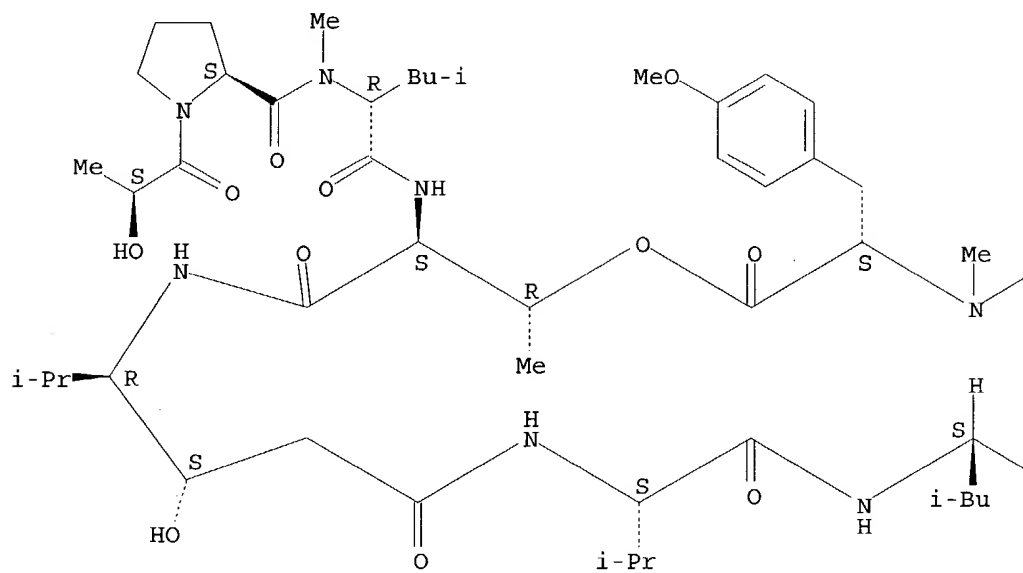
PAGE 1-B



RN 367507-56-0 HCAPLUS
CN Tamandarin B, 6-L-valine- (9CI) (CA INDEX NAME)

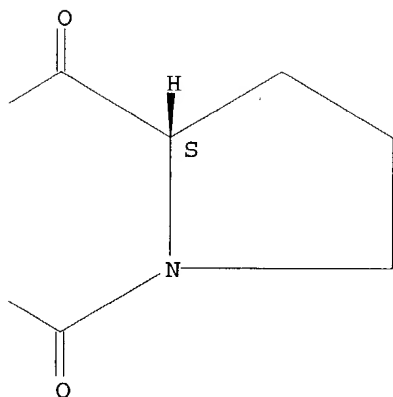
Absolute stereochemistry.

PAGE 1-A



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PAGE 1-B

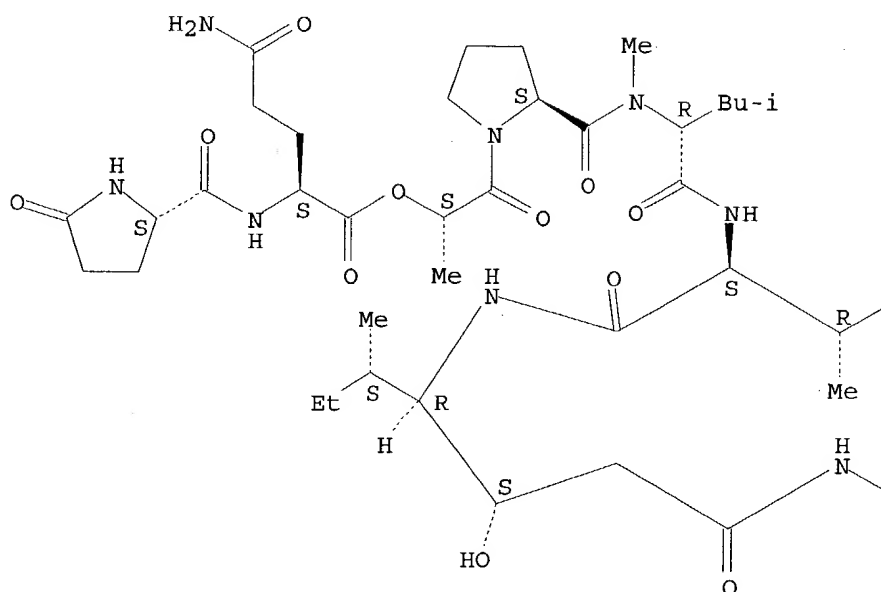


RN 367507-57-1 HCAPLUS

CN Tamandarin A, 6-L-valine-, (2'→1)-ester with 5-oxo-L-prolyl-L-glutamine (9CI) (CA INDEX NAME)

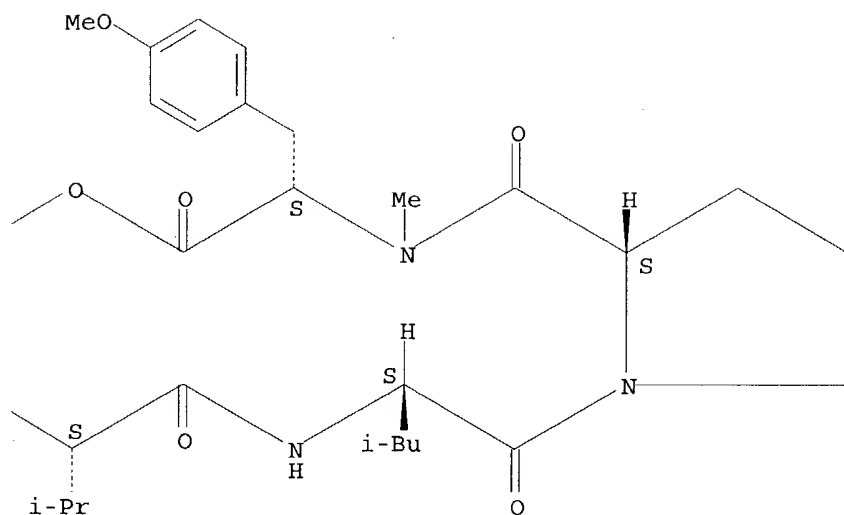
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

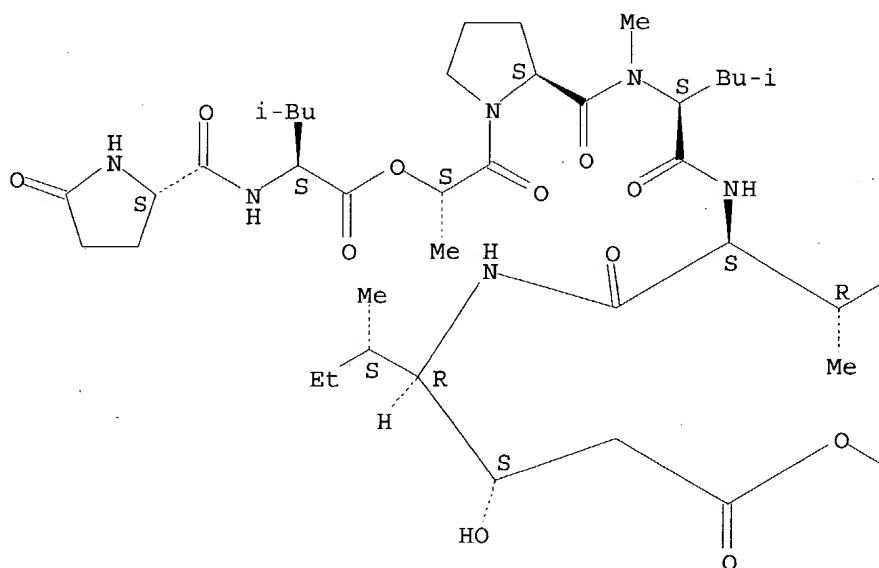


RN 367507-58-2 HCAPLUS

CN L-Tyrosine, 5-oxo-L-prolyl-L-leucyl-(2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-L-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (11→6)-lactone (9CI) (CA INDEX NAME)

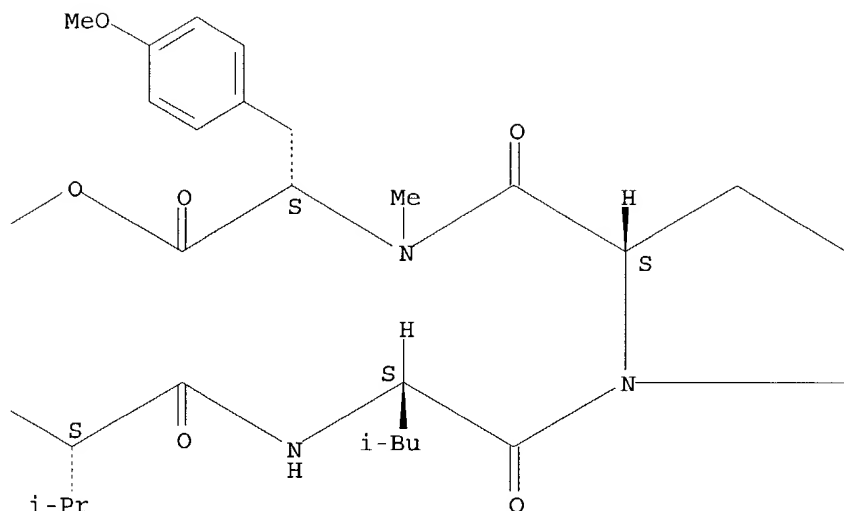
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

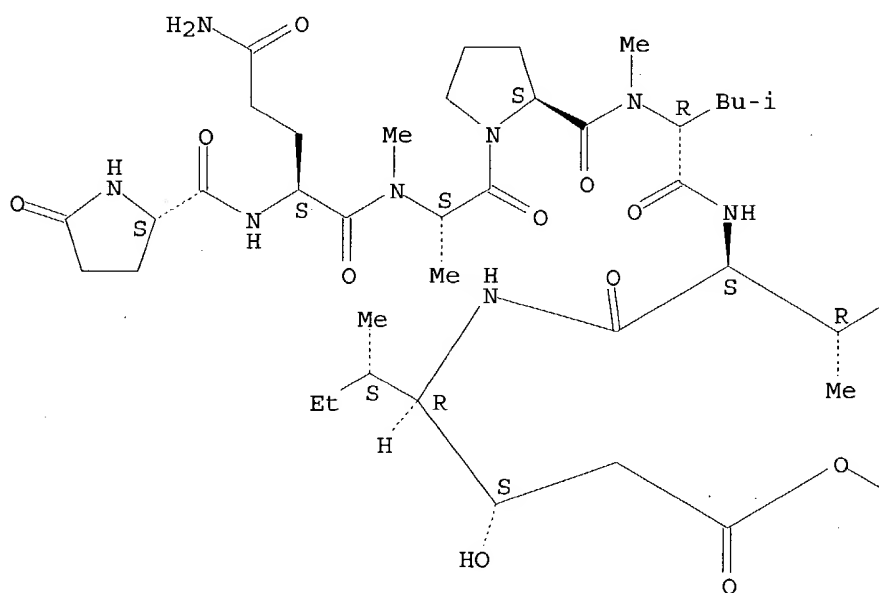


RN 367507-59-3 HCAPLUS

CN L-Tyrosine, 5-oxo-L-prolyl-L-glutaminyl-N-methyl-L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl- (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (11→6)-lactone (9CI) (CA INDEX NAME)

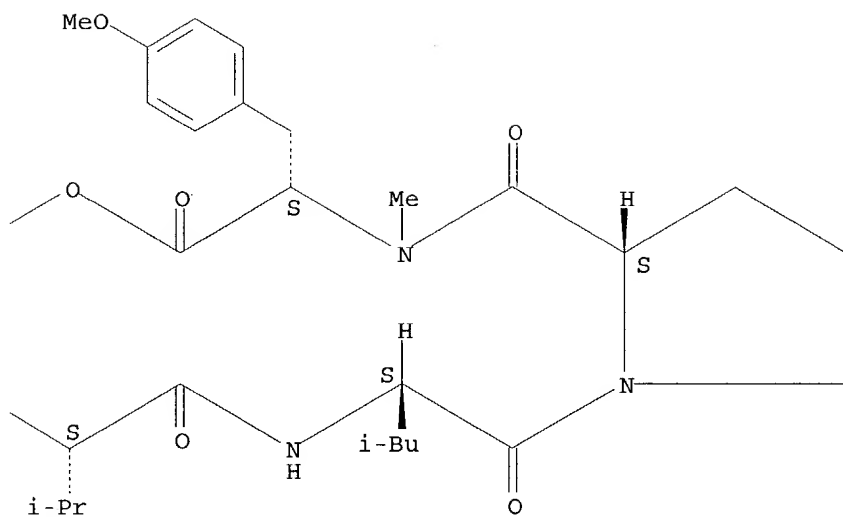
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B

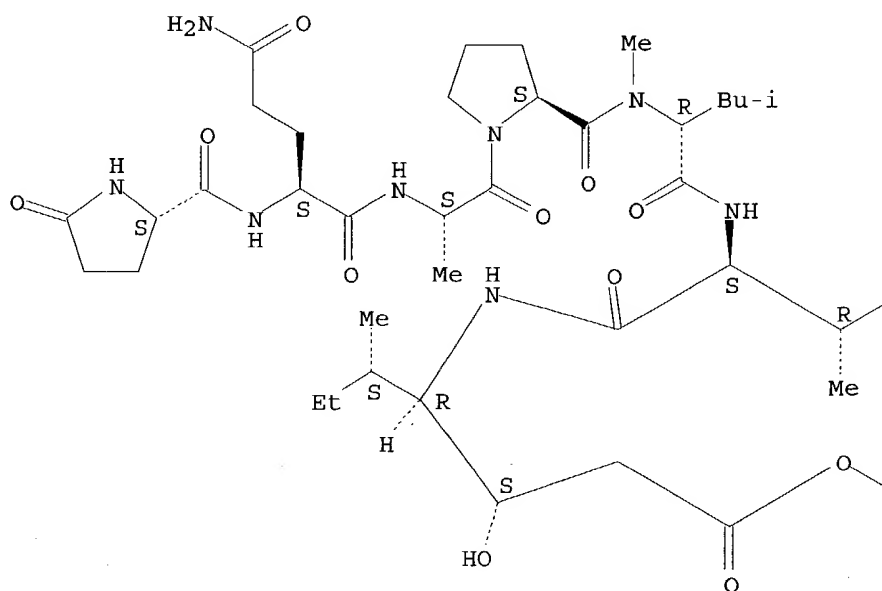


RN 367507-60-6 HCAPLUS

CN L-Tyrosine, 5-oxo-L-prolyl-L-glutaminyl-L-alanyl-L-prolyl-N-methyl-D-leucyl-L-threonyl- (3S,4R,5S) -4-amino-3-hydroxy-5-methylheptanoyl- (2S) -2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (11→6)-lactone (9CI) (CA INDEX NAME)

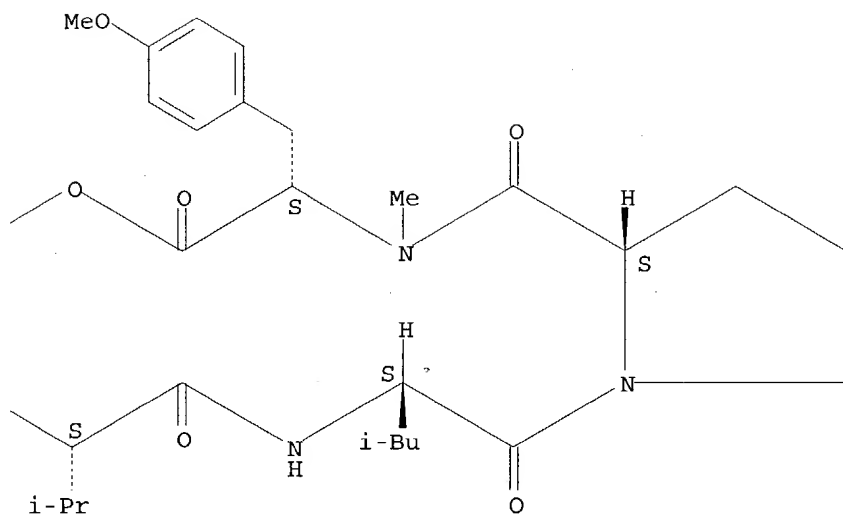
Absolute stereochemistry.

PAGE 1-A



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PAGE 1-B

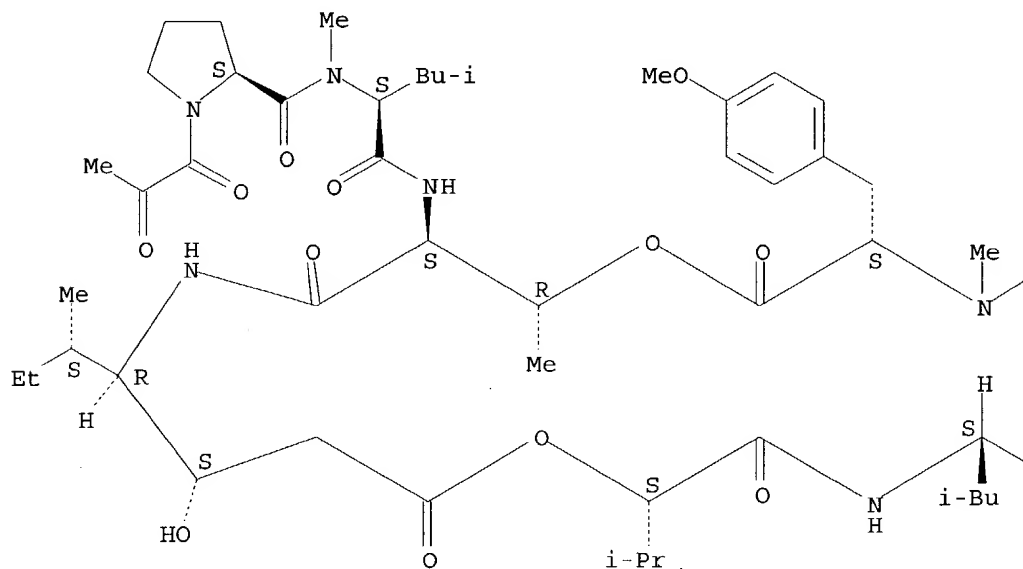


RN 367507-61-7 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-L-leucyl-L-threonyl-
 (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-
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 (CA INDEX NAME)

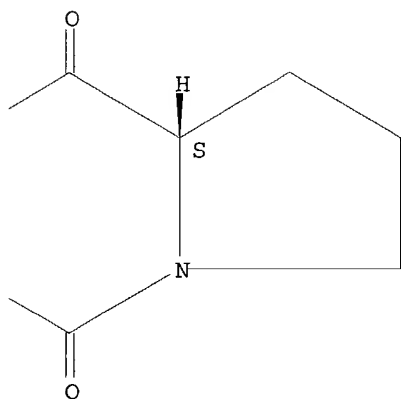
Absolute stereochemistry.

PAGE 1-A



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PAGE 1-B

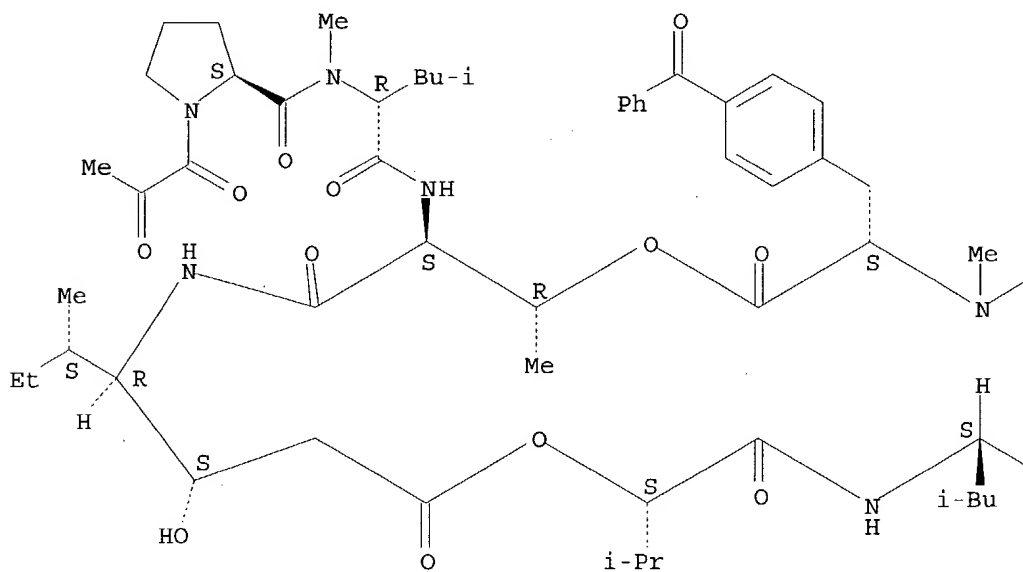


RN 367507-62-8 HCAPLUS

CN L-Phenylalanine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-4-benzoyl-N-methyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

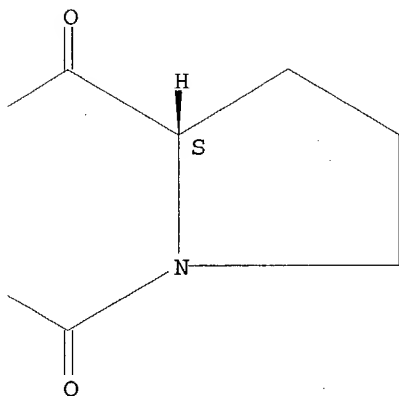
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B



RN 367507-63-9 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxybutanoyl-L-leucyl-L-prolyl-1,2,3,4-tetrahydro-7-methoxy-, (8→3)-lactone, (3S)- (9CI) (CA INDEX NAME)

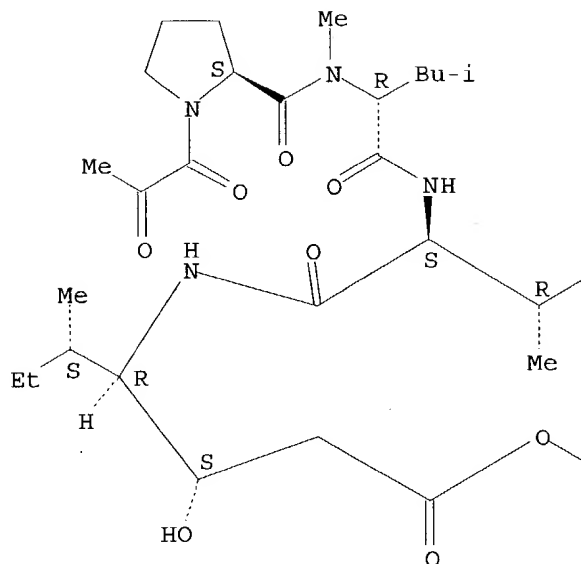
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RN 367507-64-0 HCAPLUS

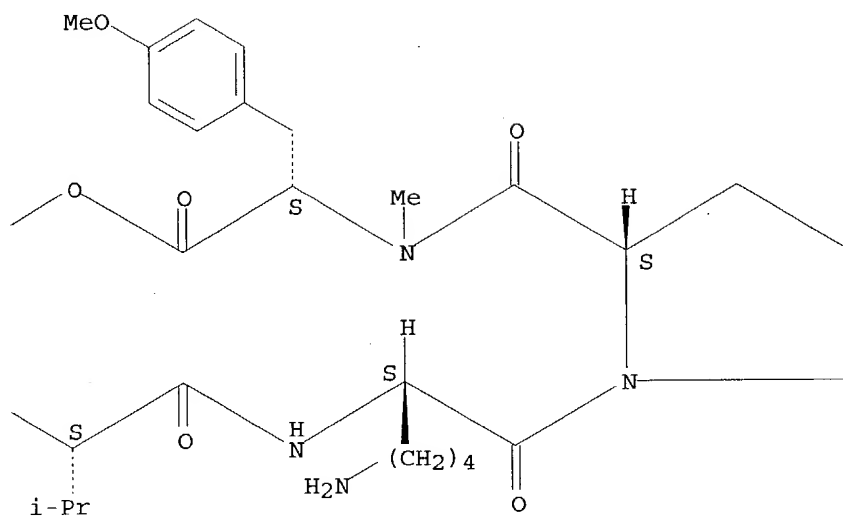
CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-lysyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



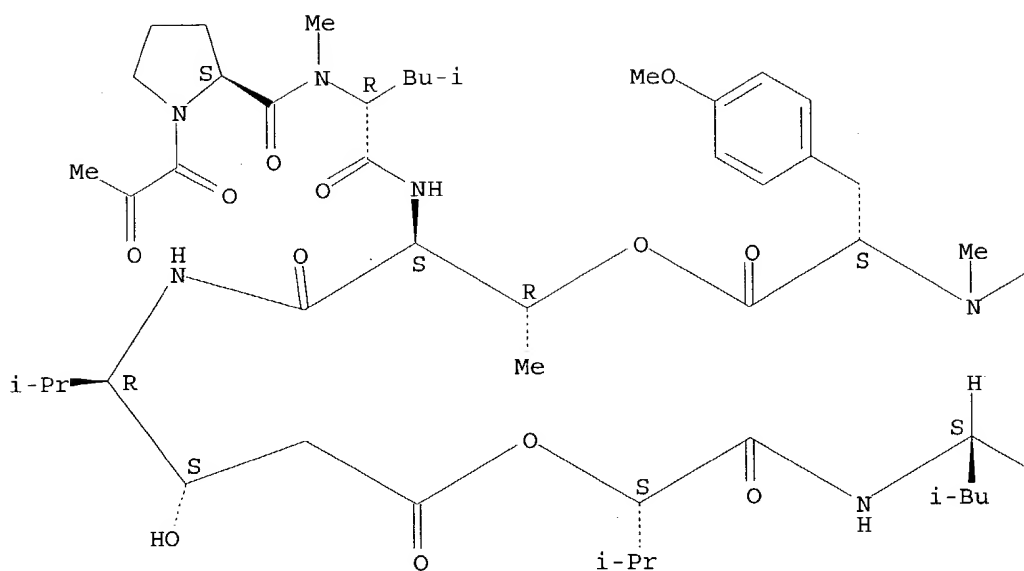
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 NAME)

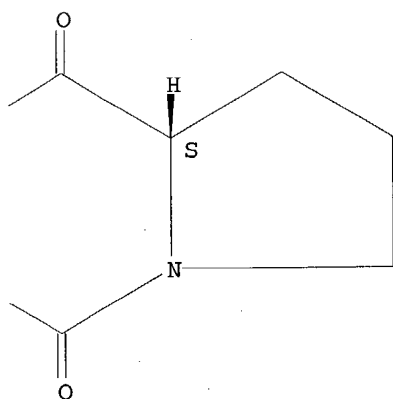
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



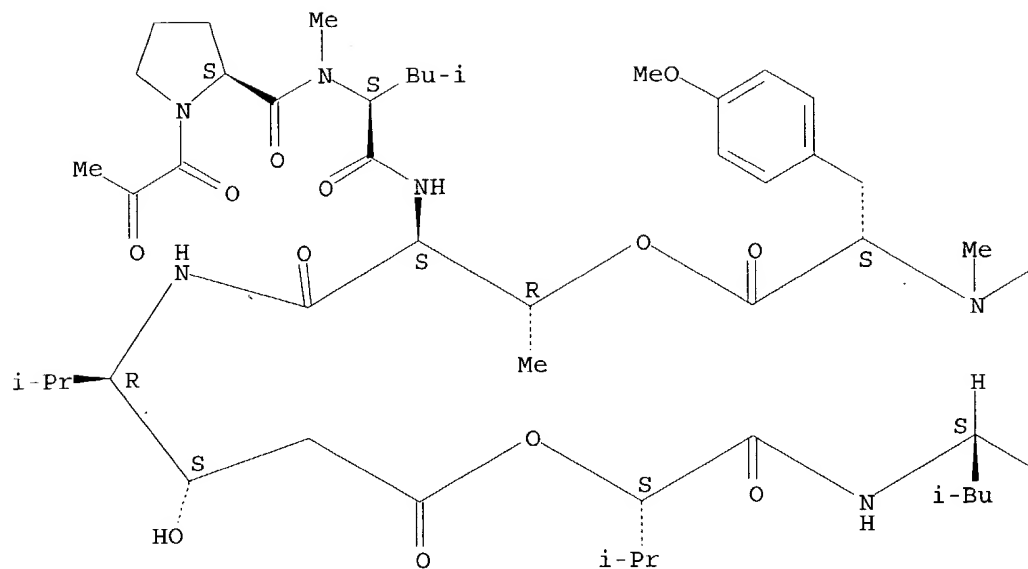
RN 367507-66-2 HCAPLUS

CN L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-L-leucyl-L-threonyl-
 (3S,4R)-4-amino-3-hydroxy-5-methylhexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-
 L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX
 NAME)

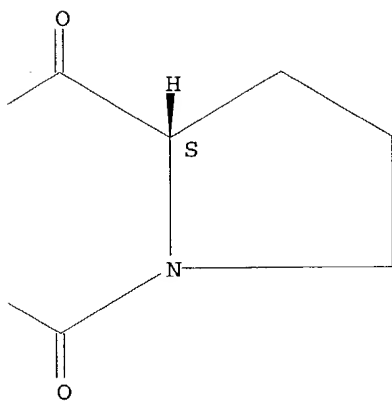
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



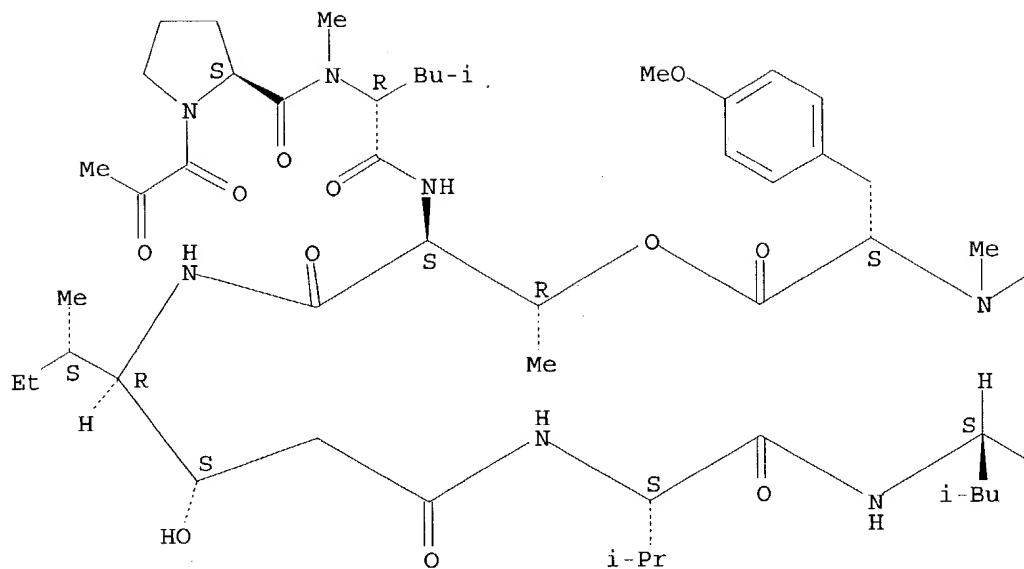
RN 367507-67-3 HCAPLUS

CN 2-9-Tamandarin A, 2-[1-(1,2-dioxopropyl)-L-proline]-6-L-valine- (9CI) (CA INDEX NAME)

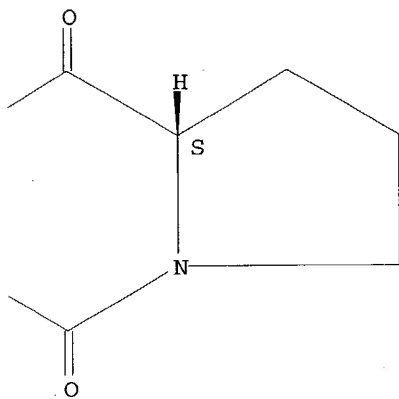
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



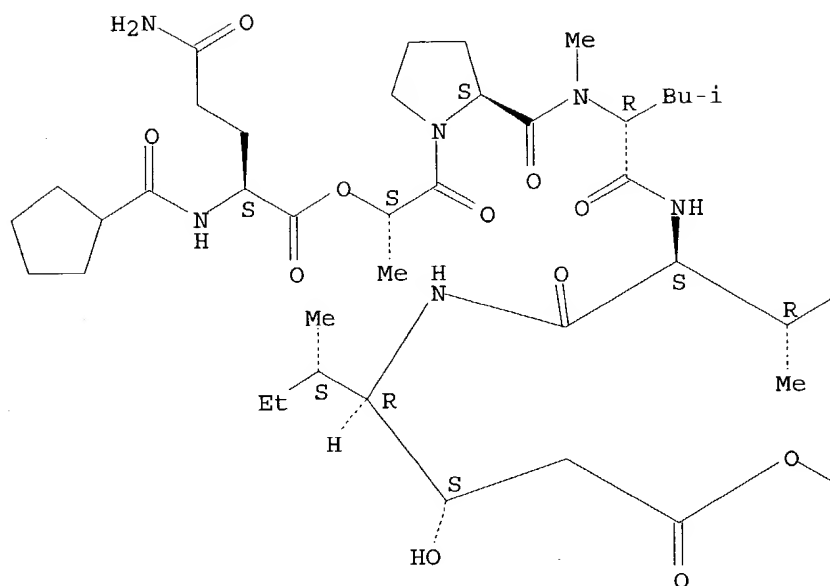
RN 367939-75-1 HCAPLUS

CN L-Tyrosine, N2-(cyclopentylcarbonyl)-L-glutaminyl-(2S)-2-hydroxypropanoyl-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (10→5)-lactone (9CI) (CA INDEX NAME)

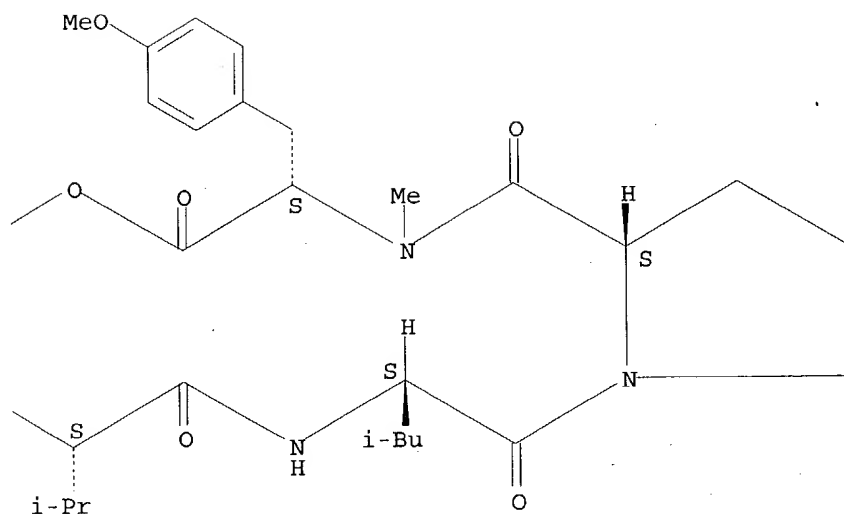
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



IT 250039-55-5P 291772-83-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tamandarin and didemnin analogs)

RN 250039-55-5 HCAPLUS

CN 4-9-Tamandarin A, N-[(1,1-dimethylethoxy)carbonyl]-5-[(3S,4R,5S)-4-amino-5-methyl-3-[[tris(1-methylethyl)silyl]oxy]heptanoic acid]- (9CI) (CA INDEX

Searched by P. Ruppel

Absolute stereochemistry.

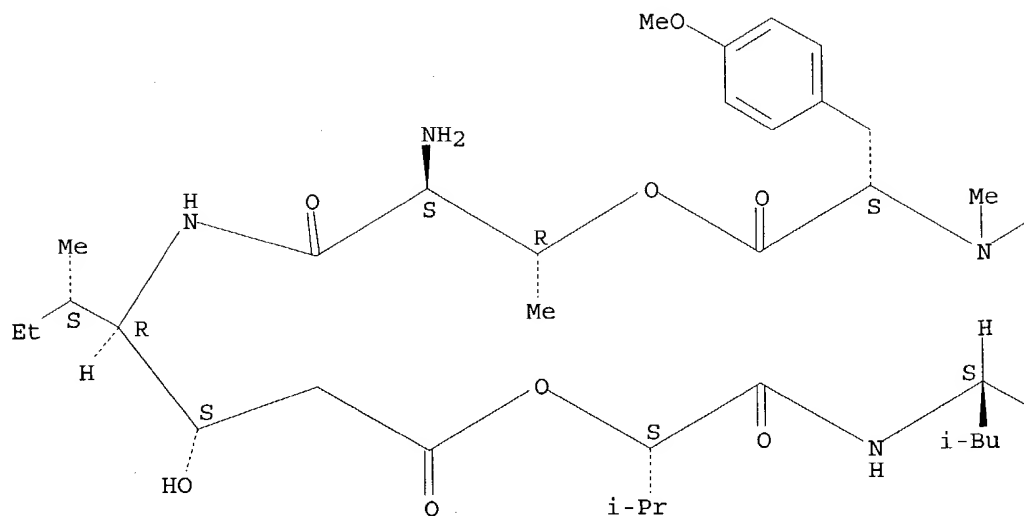
Chemical structure of compound 10, a macrocyclic peptide derivative. The structure features a 12-membered ring with various side chains including a tert-butyl ester, a 4-methoxybenzyl group, an isopropyl group, and a trimethylsilyl group. Stereochemistry is indicated with wedges and dashes.

RN 291772-83-3 HCAPLUS
CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-
2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-,
(6-1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

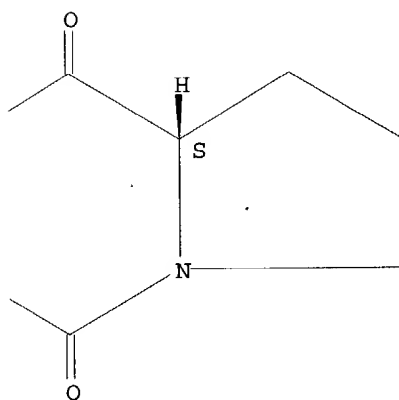
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:268658 HCAPLUS

DOCUMENT NUMBER: 135:61525

TITLE: Total syntheses and biological investigations of

tamandarins A and B and tamandarin A analogs

AUTHOR(S): Liang, Bo; Richard, David J.; Portonovo, Padma S.;

Joullie, Madeleine M.

CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA

Searched by P. Ruppel

SOURCE: Journal of the American Chemical Society (2001),
123(19), 4469-4474
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:61525
AB Tamandarins A (1) and B (2), two natural products similar in structure to didemnin B (3), were recently isolated from a Brazilian marine ascidian of the family Didemnidae. The cytotoxicity of 1 was reported to be somewhat more potent in vitro than that of 3 against various human cancer cell lines. The present account describes the first total syntheses of 1 and 2, and the syntheses of tamandarin A side chain analogs. The cytotoxicity data for these compds. show that the side chain modifications exhibit a parallel effect for both didemnins and tamandarins. This observation supports tamandarins' role as didemnins' mimic.

IT 258339-38-7P, Tamandarin B

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

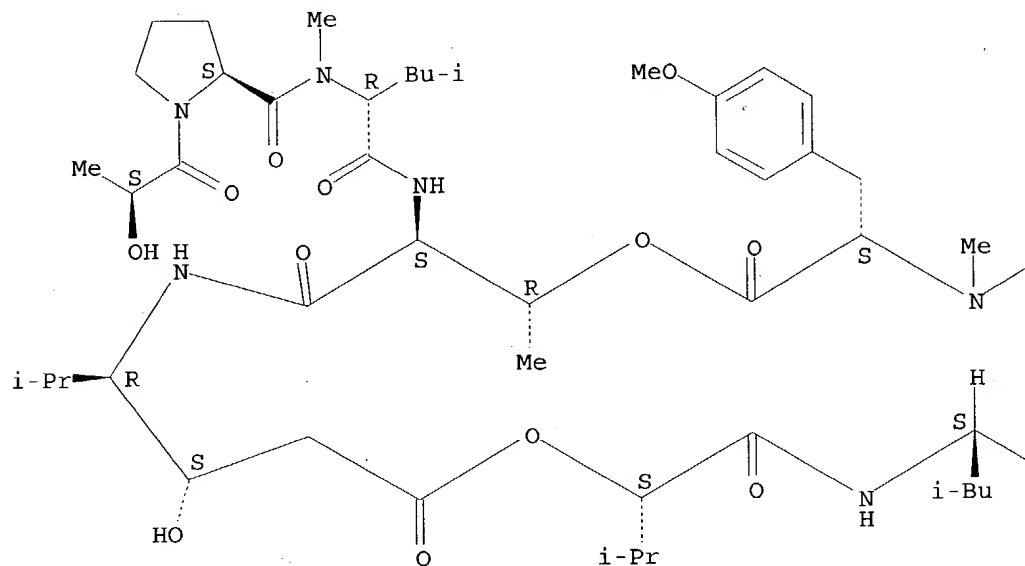
(preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)

RN 258339-38-7 HCAPLUS

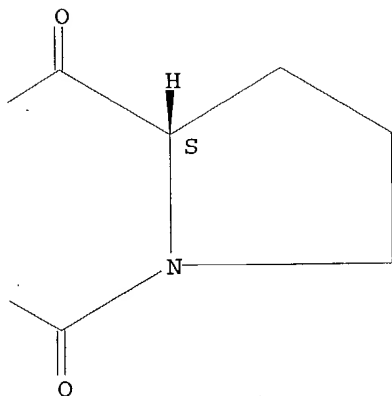
CN Tamandarin B (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



IT 291772-81-1

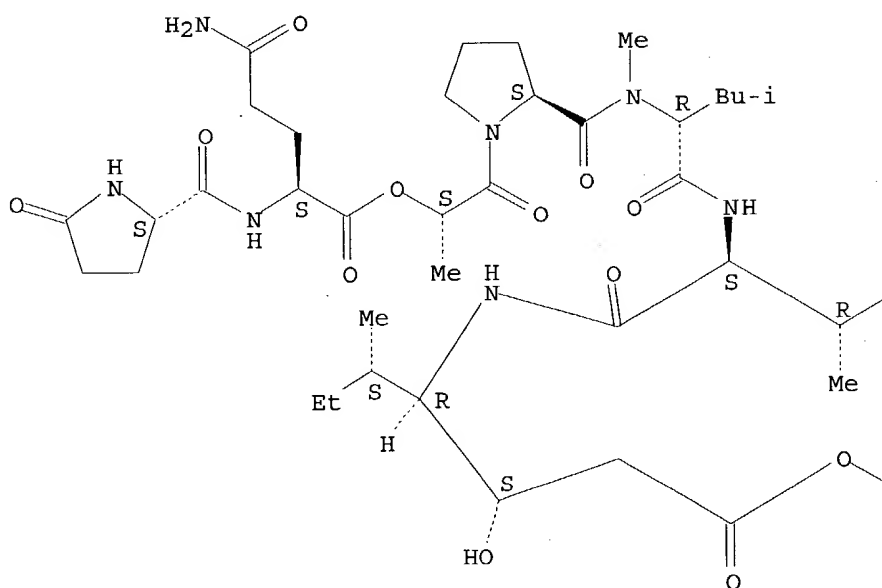
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)

RN 291772-81-1 HCAPLUS

CN Didemnin M, 8-[(2S)-2-hydroxy-3-methylbutanoic acid]- (9CI) (CA INDEX NAME)

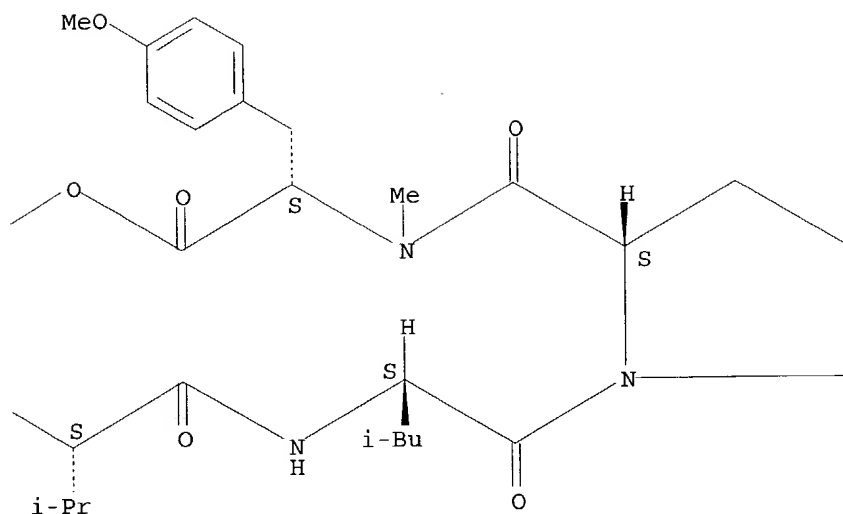
Absolute stereochemistry. Rotation (-).

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B



IT 345664-55-3P 345969-81-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

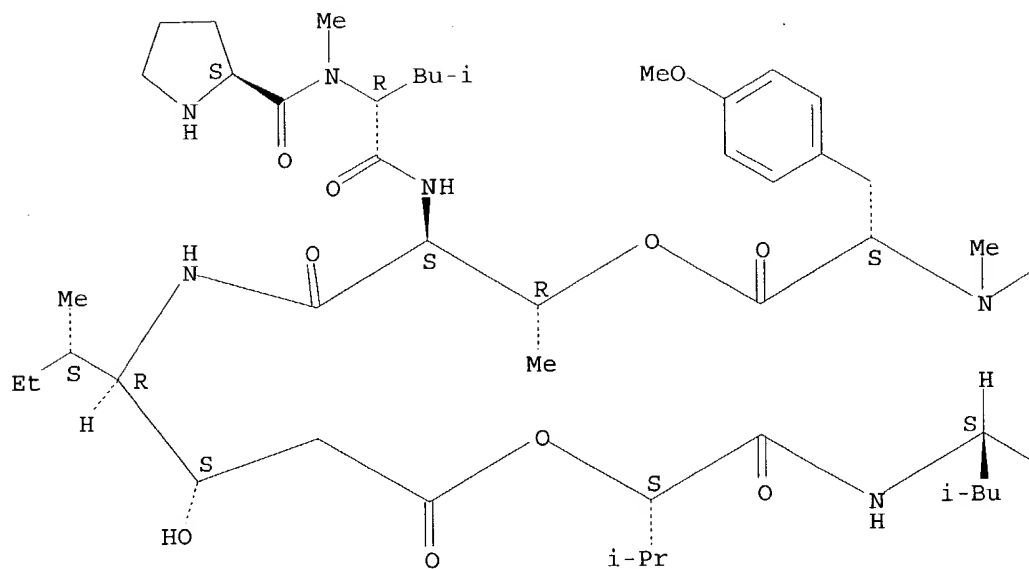
(preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)

RN 345664-55-3 HCAPLUS

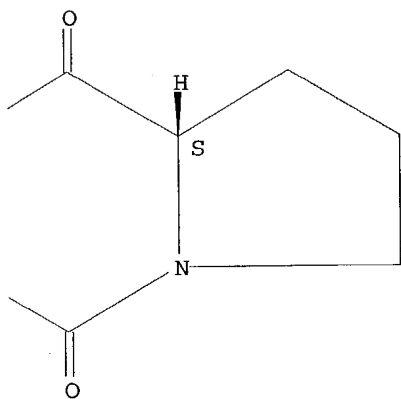
CN L-Tyrosine, L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B

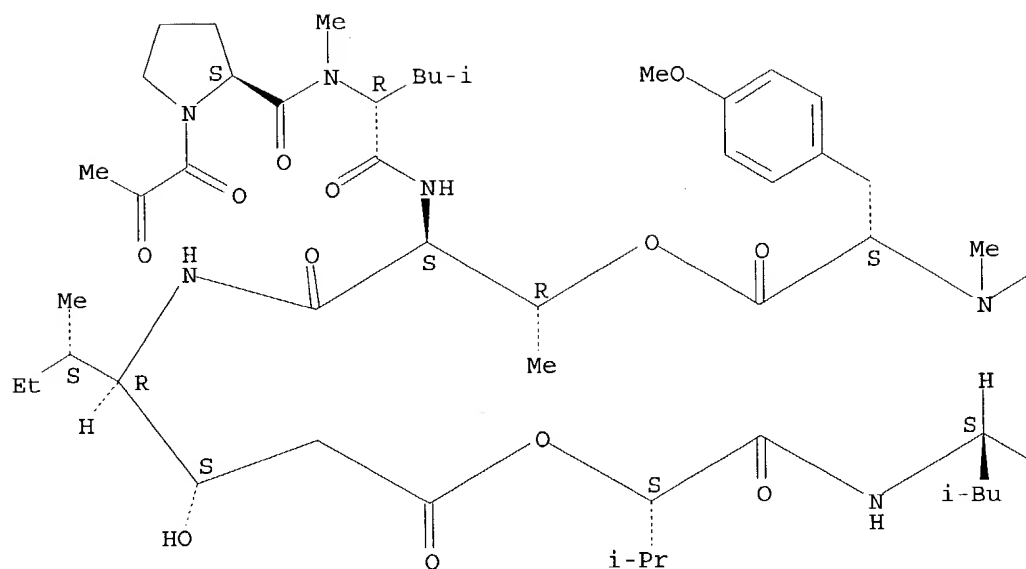


RN	345969-81-5	HCAPLUS
CN	L-Tyrosine, 1-(1,2-dioxopropyl)-L-prolyl-N-methyl-D-leucyl-L-threonyl- (3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3- methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI) (CA INDEX NAME)	

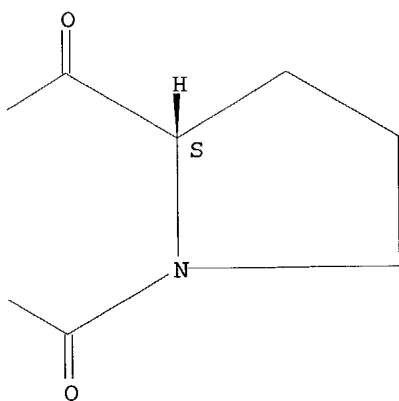
Absolute stereochemistry. Rotation (-).

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B

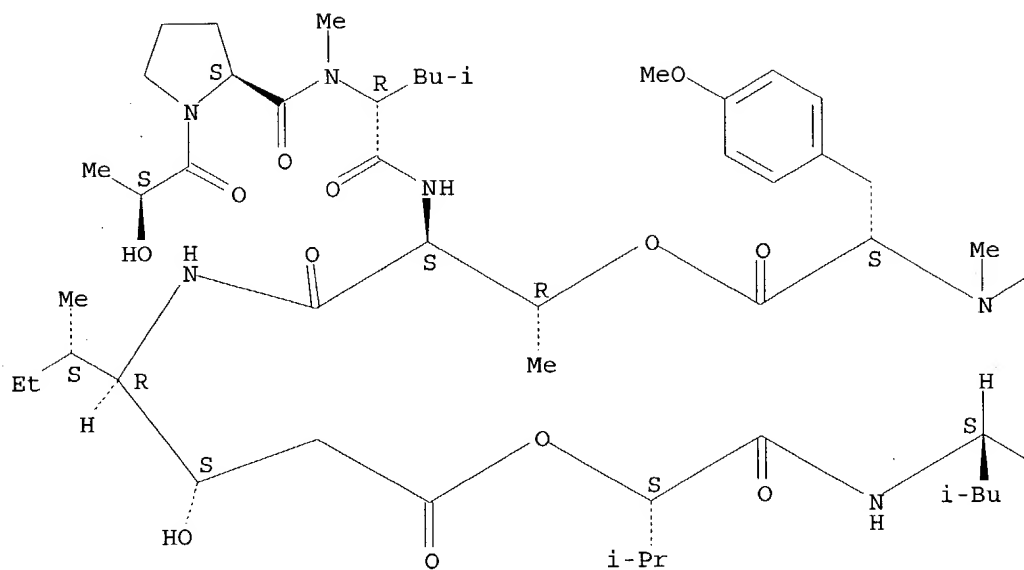


IT 250211-78-0P, Tamandarin A
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A analogs and didemnin analogs)
 RN 250211-78-0 HCAPLUS
 CN Tamandarin A (9CI) (CA INDEX NAME)

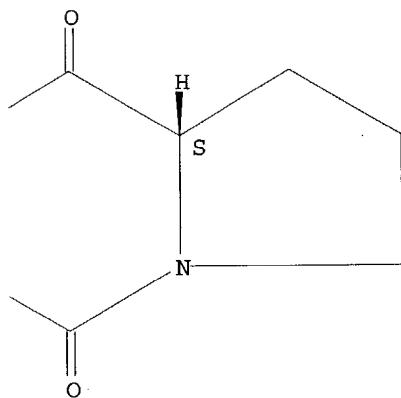
Searched by P. Ruppel

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



IT 250039-55-5P 291772-83-3P 325687-71-6P
 345664-71-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and cytotoxicity of tamandarin A, tamandarin B, tamandarin A
 analogs and didemnin analogs)

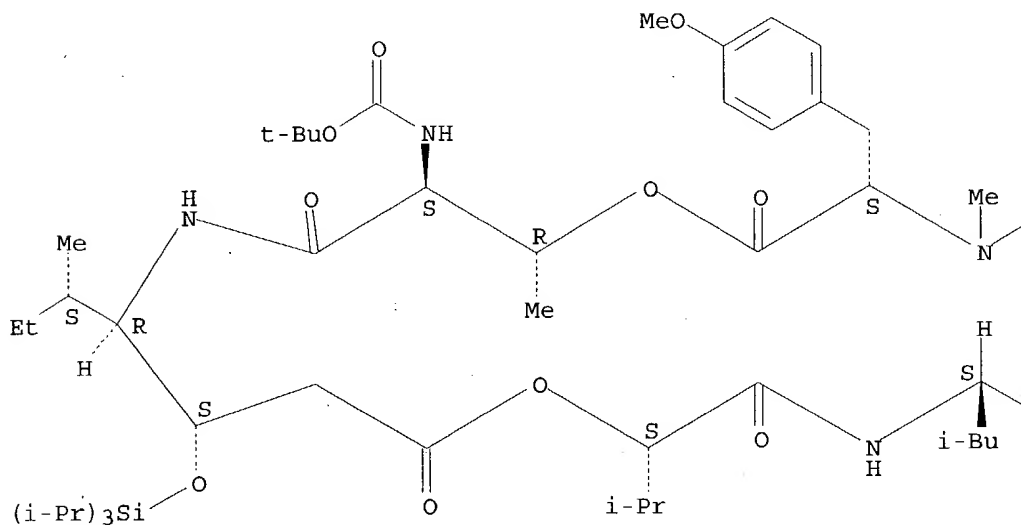
RN 250039-55-5 HCAPLUS

Searched by P. Ruppel

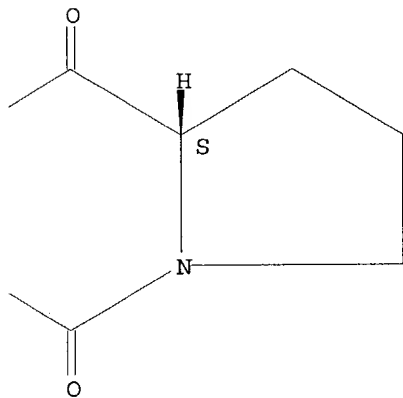
CN 4-9-Tamandarin A, N-[(1,1-dimethylethoxy)carbonyl]-5-[(3S,4R,5S)-4-amino-5-methyl-3-[[tris(1-methylethyl)silyl]oxy]heptanoic acid]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



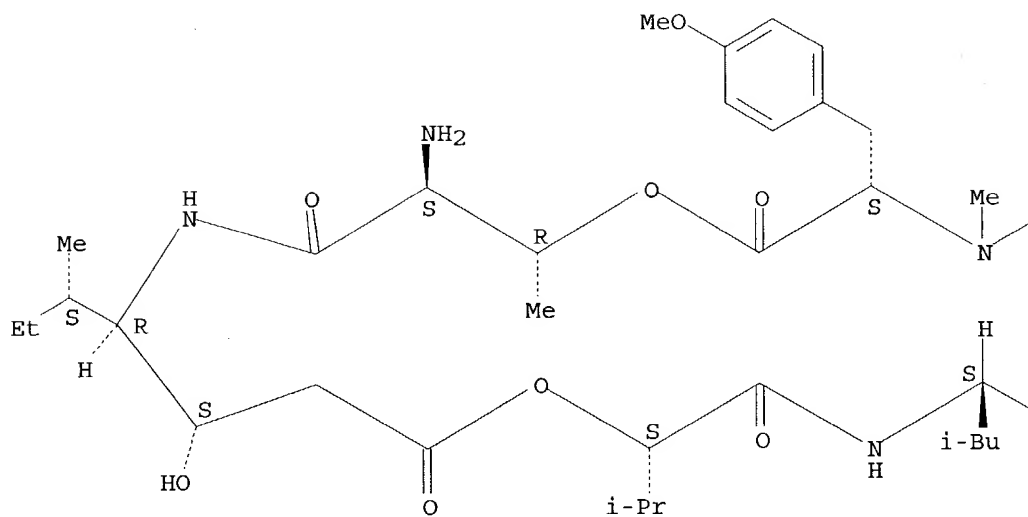
RN 291772-83-3 HCAPLUS

CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

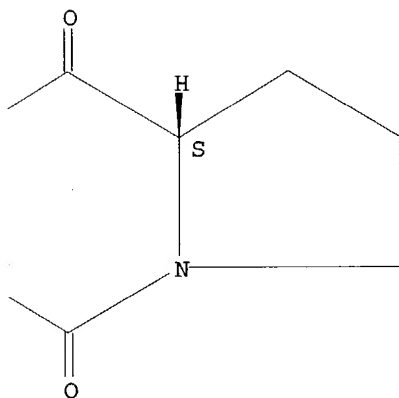
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



● HCl

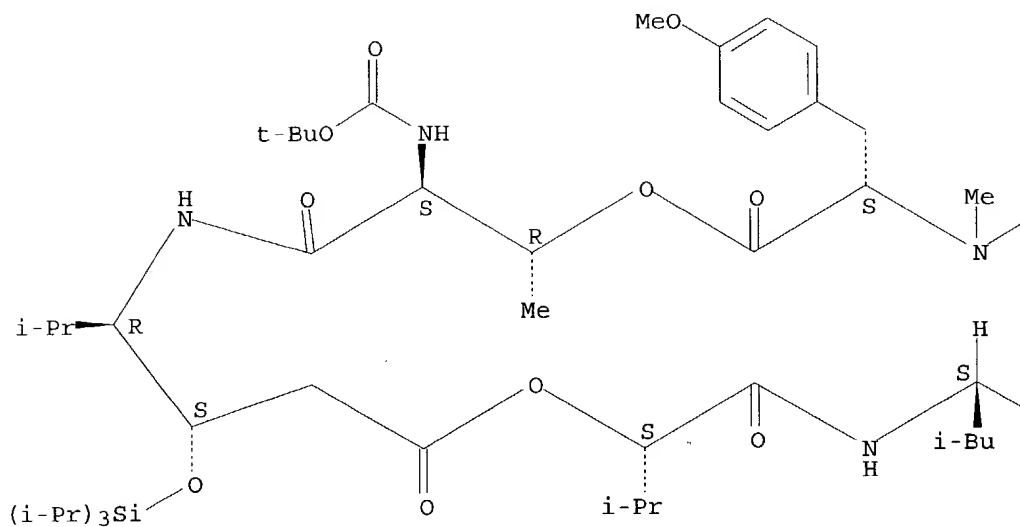
RN 325687-71-6 HCAPLUS

CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R)-4-amino-5-methyl-3-[[[tris(1-methylethyl)silyl]oxy]hexanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI)
(CA INDEX NAME)

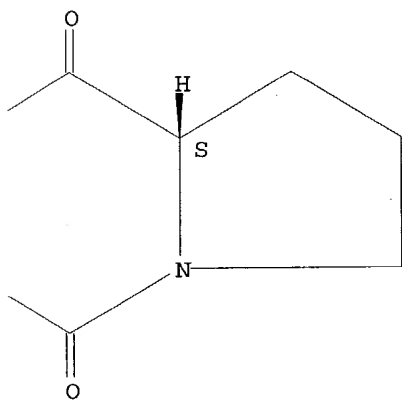
Absolute stereochemistry. Rotation (-).

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



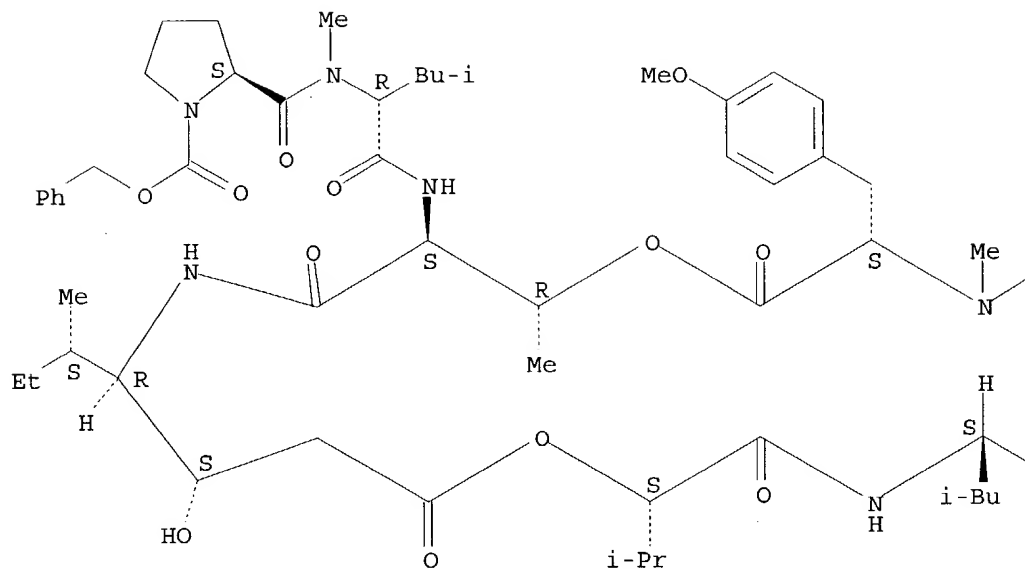
RN 345664-71-3 HCAPLUS

CN L-Tyrosine, 1-[(phenylmethoxy)carbonyl]-L-prolyl-N-methyl-D-leucyl-L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (8→3)-lactone (9CI)
(CA INDEX NAME)

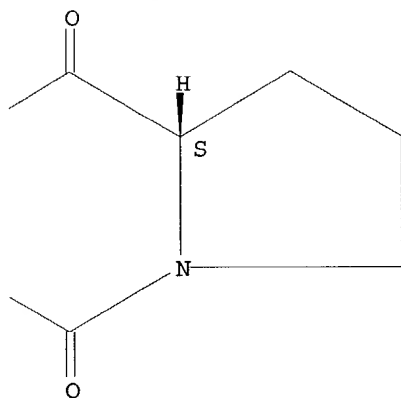
Absolute stereochemistry.

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:897488 HCAPLUS

DOCUMENT NUMBER: 134:163325

TITLE: Total synthesis of (-)-tamandarin B

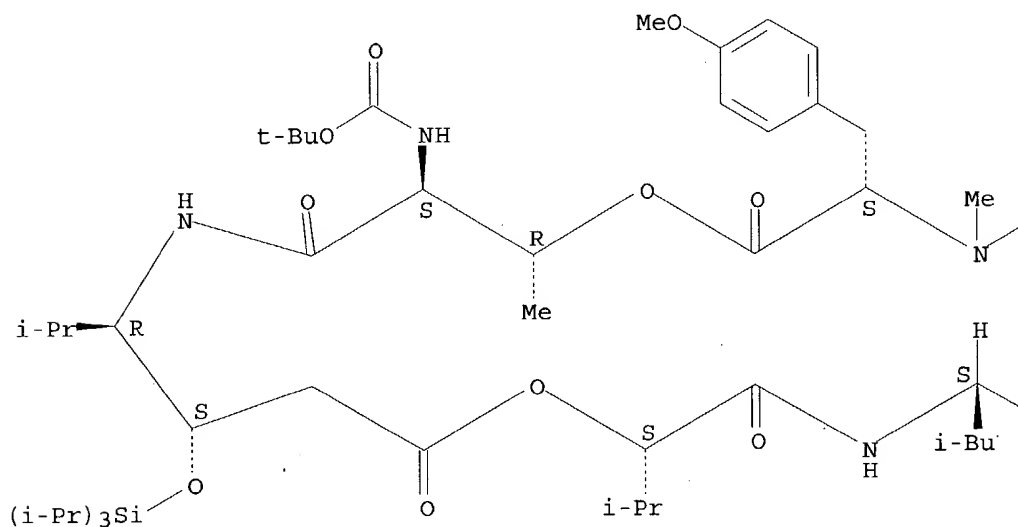
AUTHOR(S): Joullie, M. M.; Portonovo, P.; Liang, B.; Richard, D.

Searched by P. Ruppel

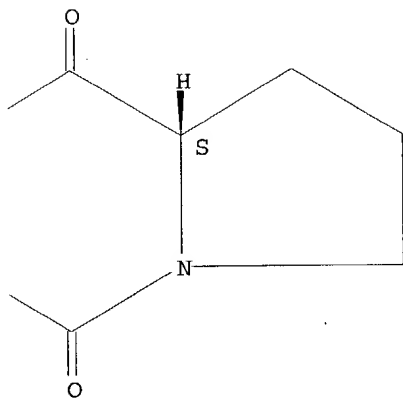
J.
 CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,
 Philadelphia, PA, 19104-6323, USA
 SOURCE: Tetrahedron Letters (2000), 41(49), 9373-9376
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:163325
 AB The synthesis of tamandarin B is described. Key steps in the synthesis of
 the macrocycle component include a diastereoselective ketone reduction, linear
 precursor formation via an activated pentafluorophenyl ester, and
 HATU-promoted cyclization. Side-chain coupling was achieved in excellent
 yield with the newly developed coupling reagent DEPBT.
 IT **325687-71-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (total synthesis of cyclic depsipeptide tamandarin B)
 RN 325687-71-6 HCAPLUS
 CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-L-threonyl-(3S,4R)-4-amino-5-
 methyl-3-[[tris(1-methylethyl)silyl]oxy]hexanoyl-(2S)-2-hydroxy-3-
 methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-, (6→1)-lactone (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



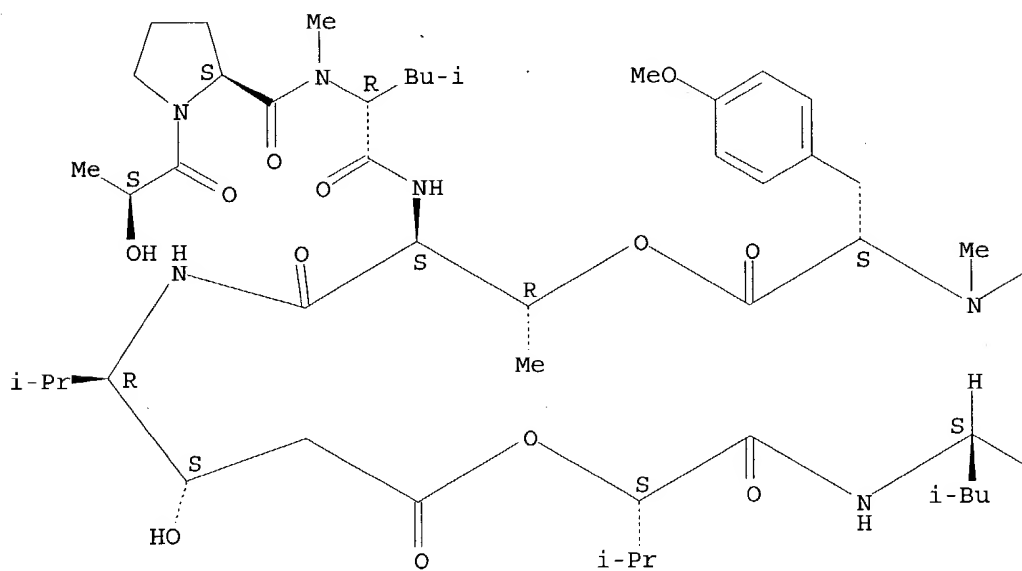
PAGE 1-B



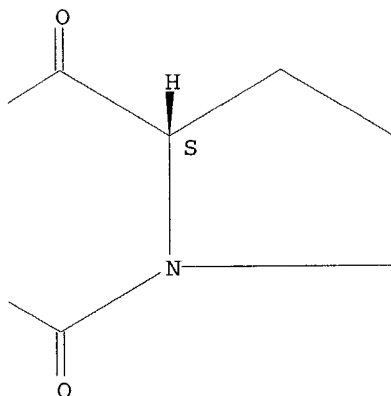
IT 258339-38-7P, Tamandarin B
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of cyclic depsipeptide tamandarin B)
RN 258339-38-7 HCAPLUS
CN Tamandarin B (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:727119 HCAPLUS

DOCUMENT NUMBER: 134:36678

TITLE: Inhibition of protein synthesis by didemnins: cell potency and SAR

AUTHOR(S): Ahuja, Deepika; Geiger, Adam; Ramanjulu, Joshi M.; Vera, Matthew D.; Sir Deshpande, Bhagyashri; Pfizenmayer, Amy; Abazeed, Mohamed; Krosky, Daniel J.; Beidler, David; Joullie, Madeleine M.; Toogood, Peter L.

CORPORATE SOURCE: Willard H. Dow Laboratory Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA

SOURCE: Journal of Medicinal Chemistry (2000), 43(22), 4212-4218

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthetic and naturally occurring didemnins are potent and specific inhibitors of protein synthesis in vitro. Structure-activity anal. indicates a requirement for the intact macrocycle; however, the smaller ring size represented by the didemnin analog, tamandarin A, is equipotent to didemnin B. Replacement of the N,O-dimethyltyrosine by a N-methylphenylalanine or N-methylleucine residue is also well-tolerated. The rank order for inhibition of protein synthesis in vitro appears to be retained in MCF-7 cells, albeit at much higher potency. This increase in potency is explained for the first time by data indicating that MCF-7 cells can accumulate didemnin B up to 2-3 orders of magnitude compared to the growth medium.

IT 250211-78-0, Tamandarin A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

Searched by P. Ruppel

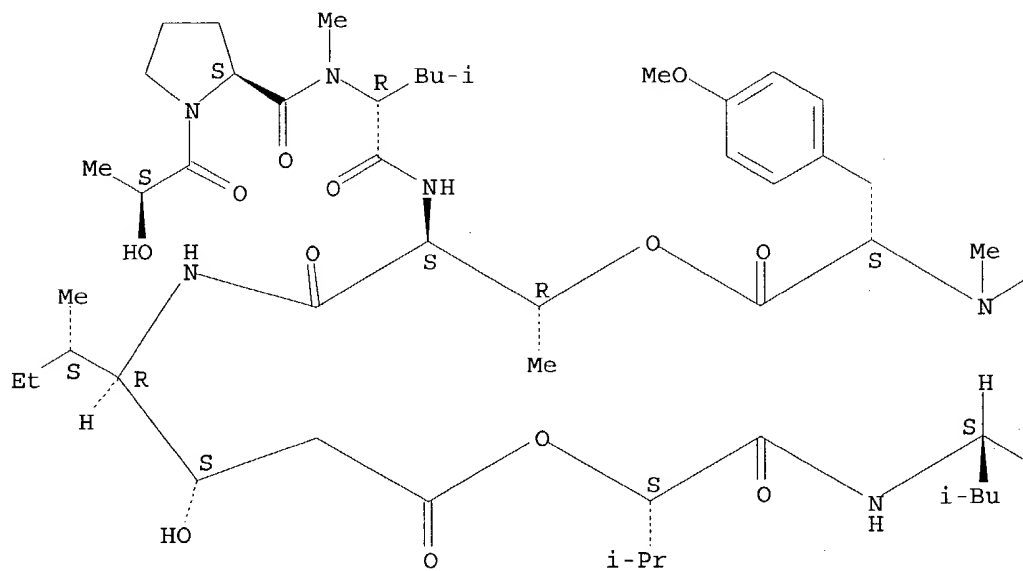
(inhibition of protein synthesis by didemnins and cell potency and SAR)

RN 250211-78-0 HCAPLUS

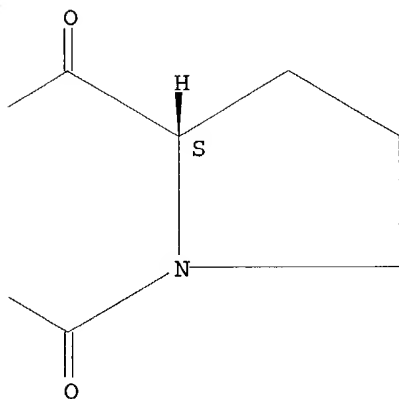
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

60

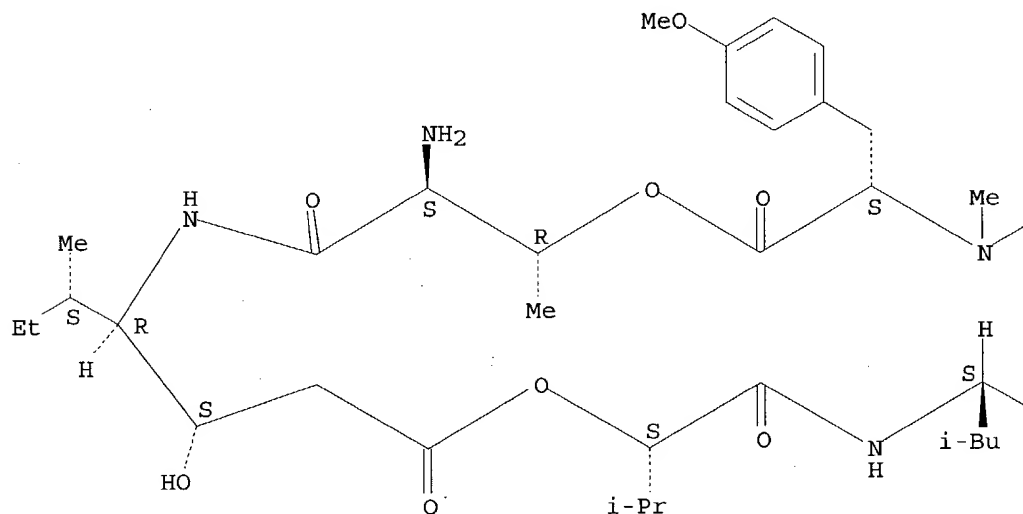
THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Searched by P. Ruppel

L62 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:417315 HCAPLUS
DOCUMENT NUMBER: 133:223009
TITLE: Total Synthesis of [(2S)-Hiv2]Didemnin M
AUTHOR(S): Liang, Bo; Vera, Matthew D.; Joullie, Madeleine M.
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania,
Philadelphia, PA, 19104-6323, USA
SOURCE: Journal of Organic Chemistry (2000), 65(15), 4762-4765
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:223009
AB The synthesis of of [(2S)-Hiv2]didemnin M (Hiv = hydroxyisovaleryl),
containing both a simplified tamandarin-type macrocycle and the more complex
side-chain of didemnin M, is reported.
IT 291772-83-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(total synthesis of (hydroxyisovaleryl)didemnin M)
RN 291772-83-3 HCAPLUS
CN L-Tyrosine, L-threonyl-(3S,4R,5S)-4-amino-3-hydroxy-5-methylheptanoyl-(2S)-
2-hydroxy-3-methylbutanoyl-L-leucyl-L-prolyl-N,O-dimethyl-,
(6→1)-lactone, monohydrochloride (9CI) (CA INDEX NAME)

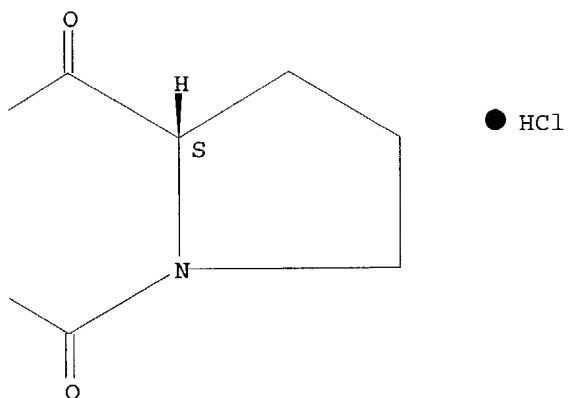
Absolute stereochemistry.

PAGE 1-A



Searched by P. Ruppel

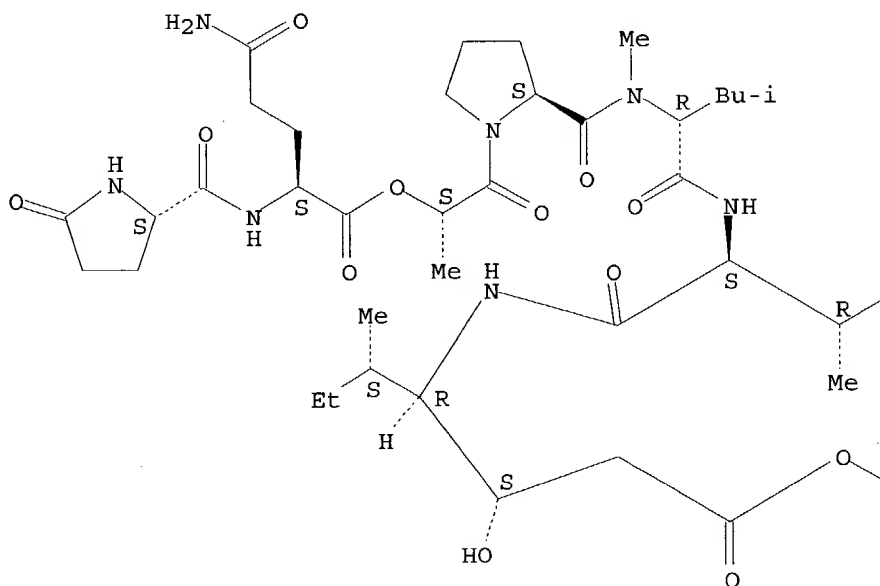
PAGE 1-B



IT 291772-81-1P, [(2S)-Hiv2]Didemnin M
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (total synthesis of (hydroxyisovaleryl)didemnin M)
 RN 291772-81-1 HCAPLUS
 CN Didemnin M, 8-[(2S)-2-hydroxy-3-methylbutanoic acid]- (9CI) (CA INDEX
 NAME)

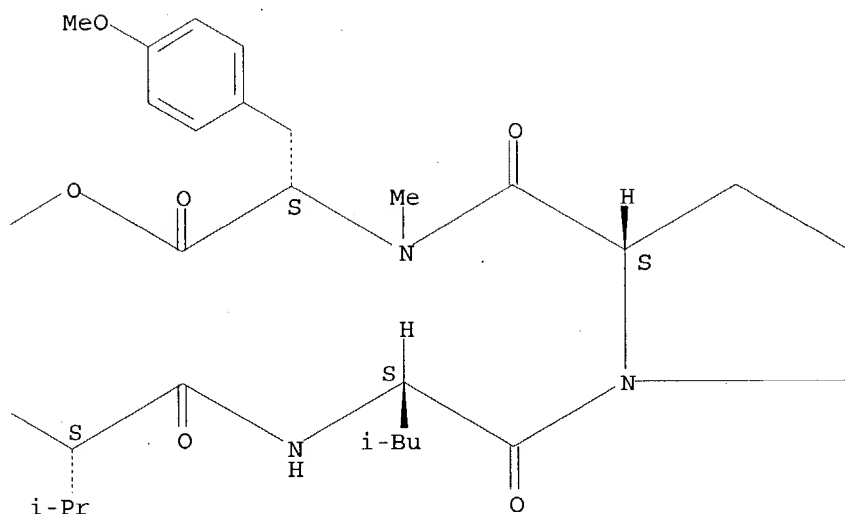
Absolute stereochemistry. Rotation (-).

PAGE 1-A



Searched by P. Ruppel

PAGE 1-B



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L62 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:816199 HCAPLUS

DOCUMENT NUMBER: 132:149193

TITLE: Tamandarins A and B: new cytotoxic depsipeptides from a Brazilian ascidian of the family Didemnidae
AUTHOR(S): Vervoort, Helene; Fenical, William; de Epifanio, Rosangela

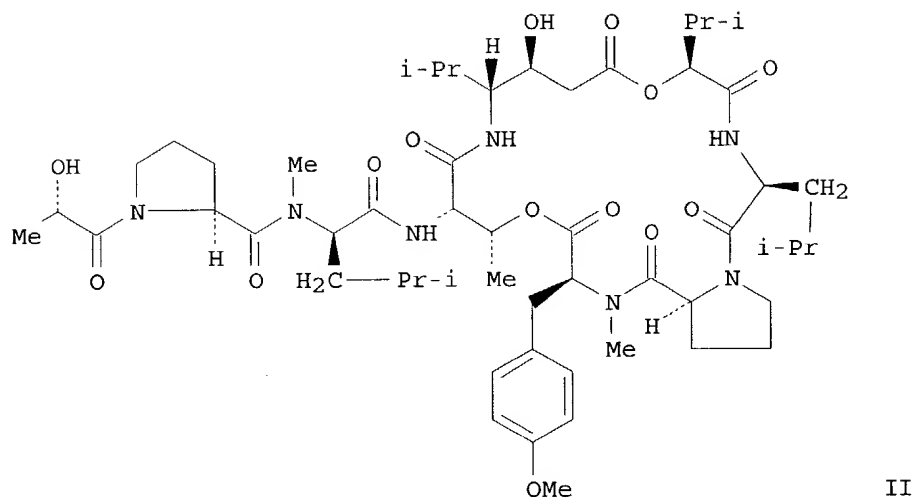
CORPORATE SOURCE: Center for Marine Biotechnology and Biomedicine
Scripps Institution of Oceanography, University of California-San Diego, La Jolla, CA, 92093-0204, USA
SOURCE: Journal of Organic Chemistry (2000), 65(3), 782-792
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The structures of two new, naturally occurring cytotoxic depsipeptides, tamandarins A(I) and B (II), are presented. The tamandarins were isolated from an unidentified Brazilian marine ascidian of the family Didemnidae. The structures of the new cytotoxins were assigned by interpretation of FABMS data and by extensive 2D NMR analyses. The absolute configurations of the tamandarins were assigned by acid and alkaline hydrolysis to yield their corresponding amino acids, which were then analyzed as their Marfey derivs. The cytotoxicity of I was evaluated against various human cancer cell lines and shown to be slightly more potent than didemnins B. A qual. discussion of the conformation of I in solution, obtained from NMR J-value data, variable temperature expts., and NOESY/ROESY data, is included.

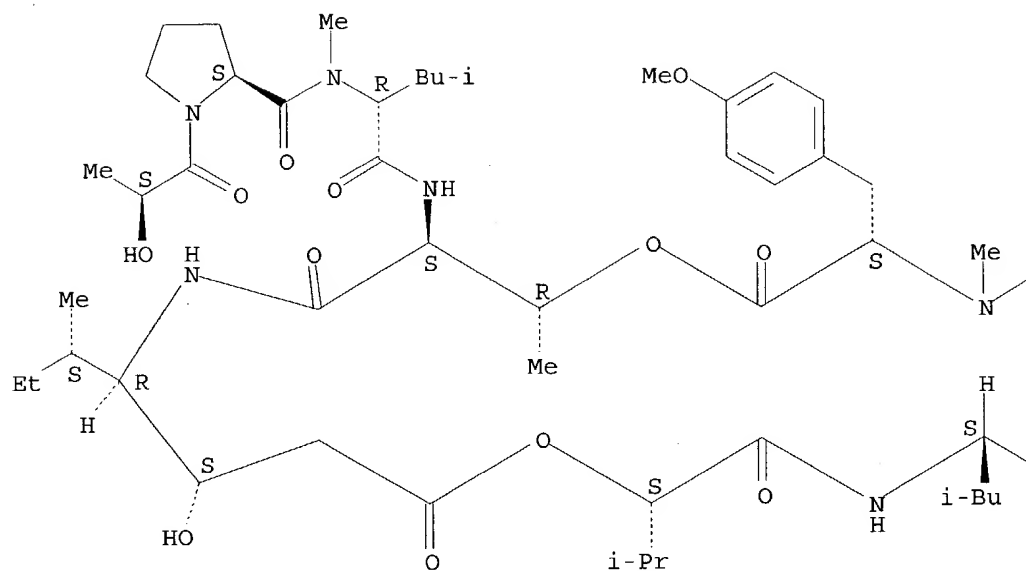
IT 250211-78-0P, Tamandarin A 258339-38-7P, Tamandarin B
 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (cytotoxic depsipeptides from ascidian)

RN 250211-78-0 HCAPLUS

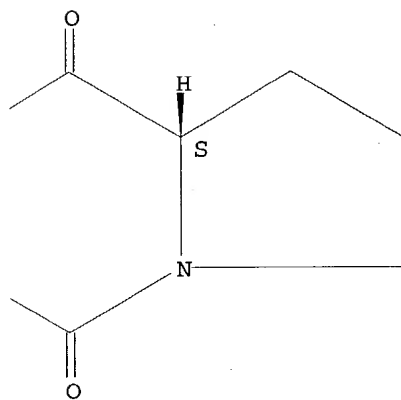
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B

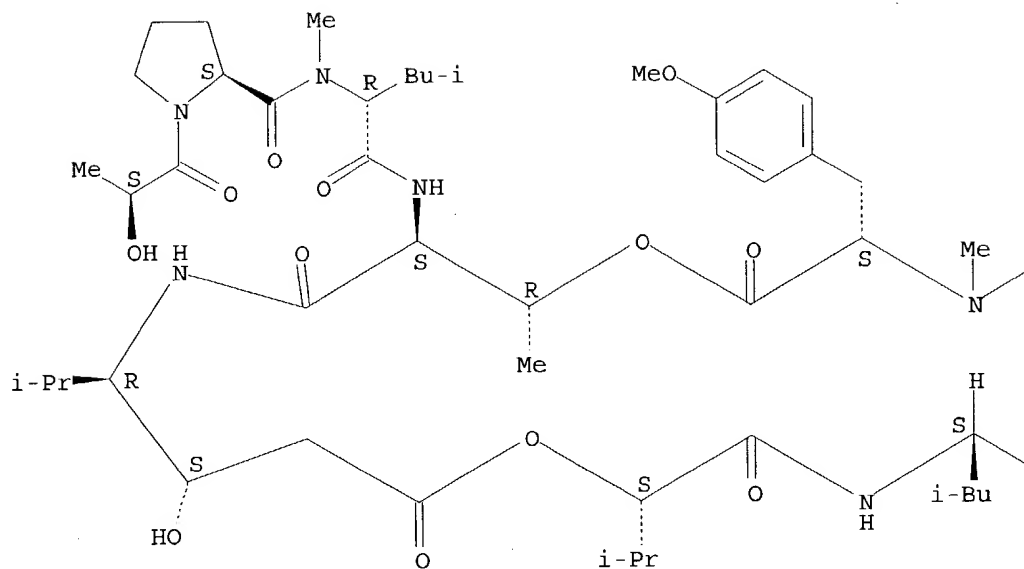


RN 258339-38-7 HCAPLUS
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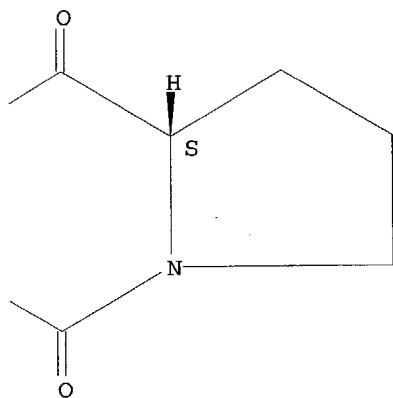
Absolute stereochemistry. Rotation (-).

Searched by P. Ruppel

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 1999:583956 HCAPLUS

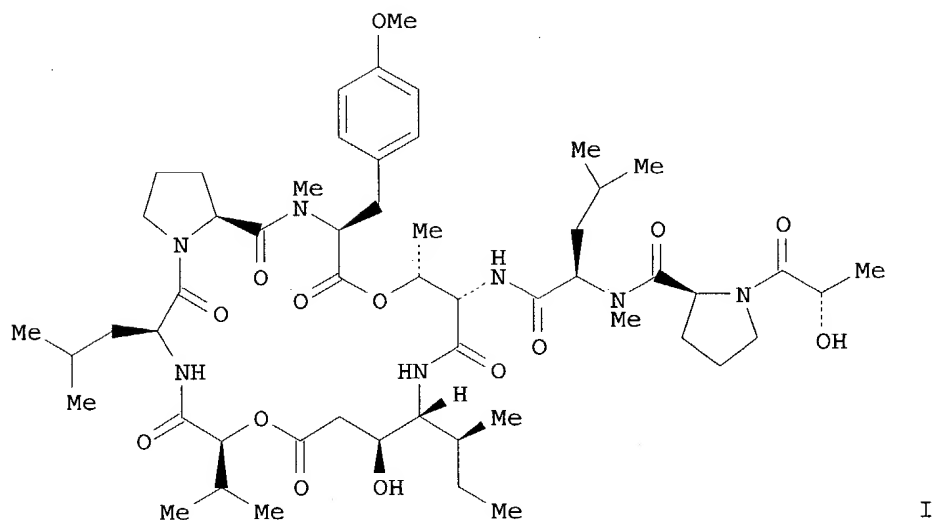
DOCUMENT NUMBER: 131:337334

TITLE: The first total synthesis of (-)-Tamandarin A

AUTHOR(S): Liang, Bo; Portonovo, Padma; Vera, Matthew D.; Xiao,

Searched by P. Ruppel

CORPORATE SOURCE: Dong, Joullie, Madeleine M.
 Department of Chemistry, University of Pennsylvania,
 Philadelphia, PA, 19104-6323, USA
 SOURCE: Organic Letters (1999), 1(8), 1319-1322
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Tamandarin A (I), a newly isolated natural product similar in structure to didemnin B, was shown to be somewhat more active in vitro than didemnin B against pancreatic carcinoma with an ED50 value 1.5 to 2 ng/mL. The first total synthesis of I is reported here. The key steps include a practical stereoselective synthesis of the α -hydroxyisovaleryl-isostatine unit, high-yielding linear precursor formation, a successful macrocyclization, and coupling of the macrocycle with the side chain to afford I.

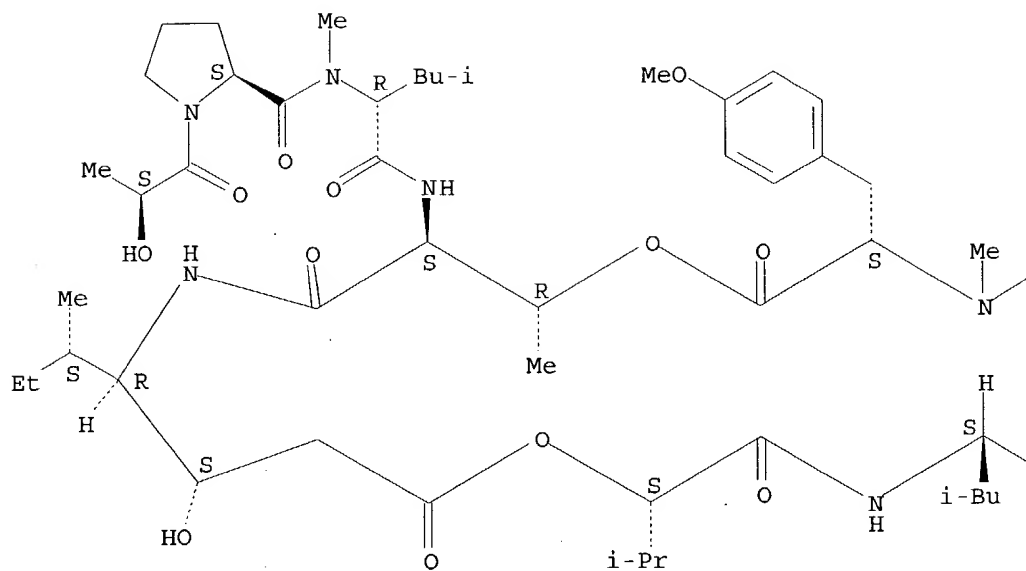
IT **250211-78-0P**, Tamandarin A
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (total synthesis of (-)-Tamandarin A, a naturally occurring anticancer cyclic depsipeptide)

RN 250211-78-0 HCAPLUS

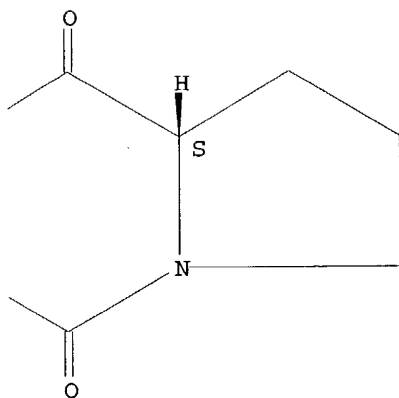
CN Tamandarin A (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 1-B



IT 250039-55-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(total synthesis of (-)-Tamandarin A, a naturally occurring anticancer cyclic depsipeptide)

RN 250039-55-5 HCAPLUS

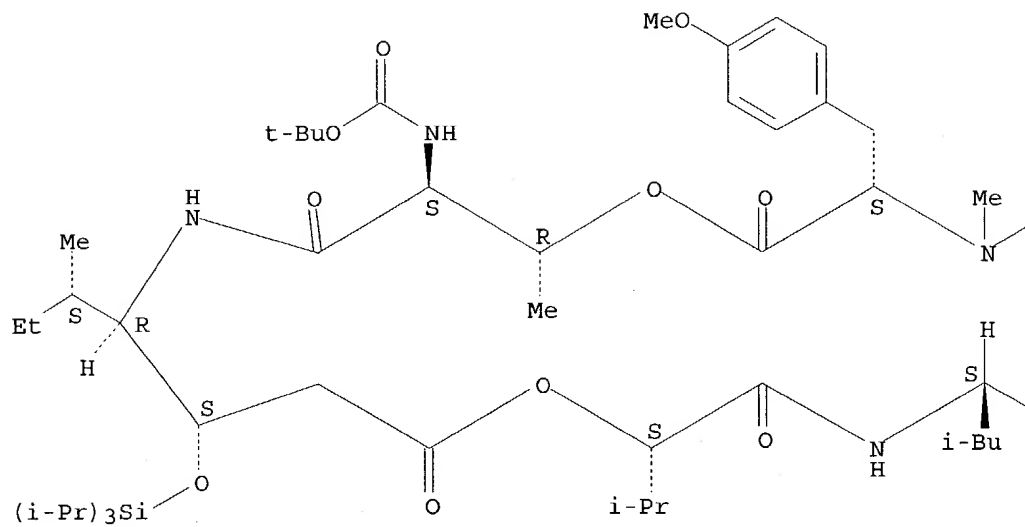
CN 4-9-Tamandarin A, N-[(1,1-dimethylethoxy)carbonyl]-5-[(3S,4R,5S)-4-amino-5-methyl-3-[[tris(1-methylethyl)silyl]oxy]heptanoic acid]- (9CI) (CA INDEX

Searched by P. Ruppel

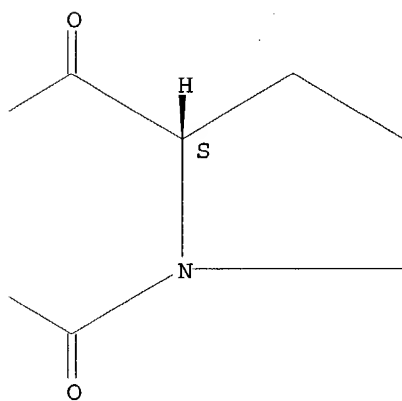
NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

26

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'HOME' ENTERED AT 17:09:37 ON 21 APR 2004

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